



## wwPDB EM Validation Summary Report ⓘ

Apr 14, 2025 – 02:11 pm BST

PDB ID : 9EYS / pdb\_00009eys  
EMDB ID : EMD-50063  
Title : Structure of Far-Red Photosystem I from *C. thermalis* PCC 7203  
Authors : Consoli, G.; Tufail, F.; Murray, J.W.; Fantuzzi, A.; Rutherford, A.W.  
Deposited on : 2024-04-09  
Resolution : 2.01 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev117  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.42



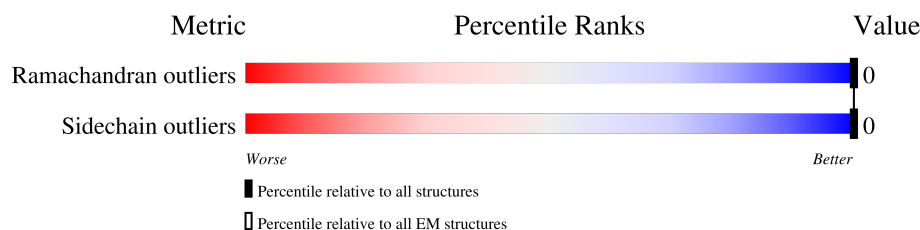
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

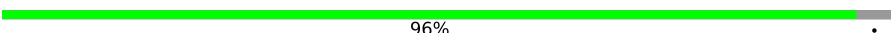
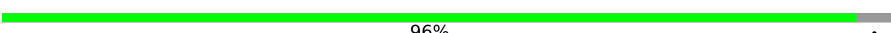
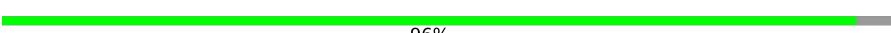
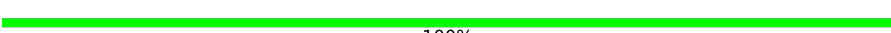





The reported resolution of this entry is 2.01 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

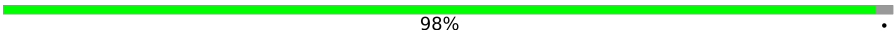
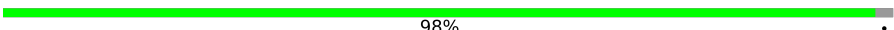
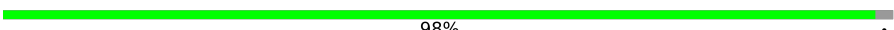
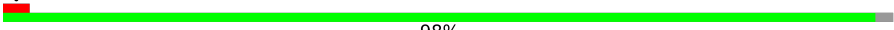
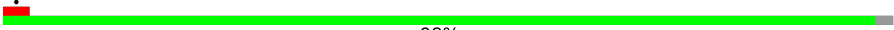





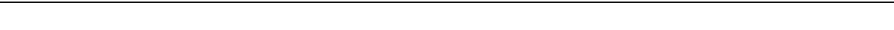

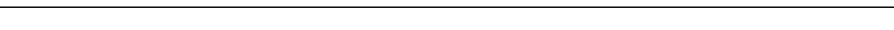
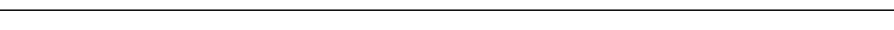
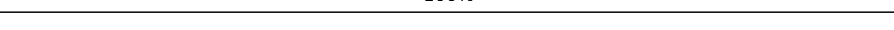
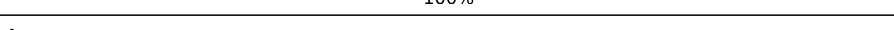
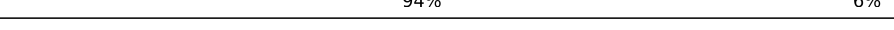
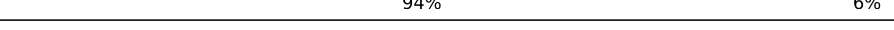
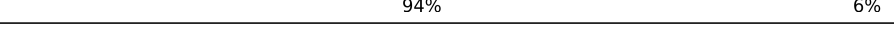
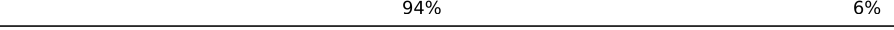
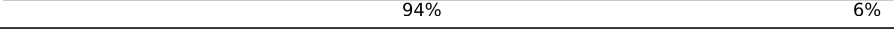
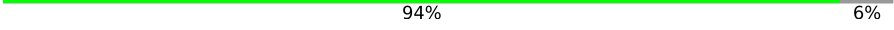
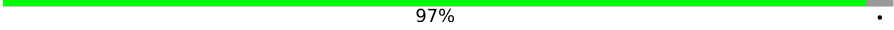
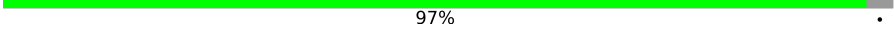
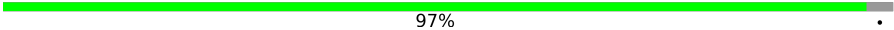
The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	782	 96% .
1	N	782	 96% .
1	a	782	 96% .
2	B	740	 100%
2	O	740	 100%
2	b	740	 100%
3	C	81	 99% .
3	P	81	 99% .
3	c	81	 99% .

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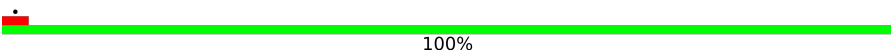

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Mol	Chain	Length	Quality of chain
4	D	142	 98% .
4	Q	142	 98% .
4	d	142	 98% .
5	E	66	 98% .
5	R	66	 98% .
5	e	66	 98% .
6	F	161	 85% 15%
6	S	161	 85% 15%
6	f	161	 85% 15%
7	I	51	 82% 18%
7	T	51	 82% 18%
7	g	51	 82% 18%
8	J	46	 100%
8	U	46	 100%
8	h	46	 100%
9	K	80	 94% 6%
9	V	80	 94% 6%
9	i	80	 94% 6%
10	L	183	 94% 6%
10	W	183	 94% 6%
10	j	183	 94% 6%
11	M	32	 97% .
11	Y	32	 97% .
11	k	32	 97% .
12	X	29	 100%

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Mol	Chain	Length	Quality of chain
12	Z	29	 100%
12	1	29	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CL0	A	801	X	-	-	-
13	CL0	N	801	X	-	-	-
13	CL0	a	801	X	-	-	-
15	CLA	A	803	X	-	-	-
15	CLA	A	804	X	-	-	-
15	CLA	A	805	X	-	-	-
15	CLA	A	806	X	-	-	-
15	CLA	A	807	X	-	-	-
15	CLA	A	808	X	-	-	-
15	CLA	A	809	X	-	-	-
15	CLA	A	810	X	-	-	-
15	CLA	A	811	X	-	-	-
15	CLA	A	812	X	-	-	-
15	CLA	A	813	X	-	-	-
15	CLA	A	814	X	-	-	-
15	CLA	A	815	X	-	-	-
15	CLA	A	816	X	-	-	-
15	CLA	A	817	X	-	-	-
15	CLA	A	818	X	-	-	-
15	CLA	A	819	X	-	-	-
15	CLA	A	820	X	-	-	-
15	CLA	A	821	X	-	-	-
15	CLA	A	822	X	-	-	-
15	CLA	A	823	X	-	-	-
15	CLA	A	825	X	-	-	-
15	CLA	A	827	X	-	-	-
15	CLA	A	828	X	-	-	-
15	CLA	A	829	X	-	-	-
15	CLA	A	830	X	-	-	-
15	CLA	A	831	X	-	-	-
15	CLA	A	832	X	-	-	-
15	CLA	A	833	X	-	-	-
15	CLA	A	834	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	A	835	X	-	-	-
15	CLA	A	836	X	-	-	-
15	CLA	A	837	X	-	-	-
15	CLA	A	838	X	-	-	-
15	CLA	A	839	X	-	-	-
15	CLA	A	840	X	-	-	-
15	CLA	A	841	X	-	-	-
15	CLA	A	842	X	-	-	-
15	CLA	A	856	X	-	-	-
15	CLA	B	801	X	-	-	-
15	CLA	B	802	X	-	-	-
15	CLA	B	803	X	-	-	-
15	CLA	B	804	X	-	-	-
15	CLA	B	805	X	-	-	-
15	CLA	B	806	X	-	-	-
15	CLA	B	807	X	-	-	-
15	CLA	B	808	X	-	-	-
15	CLA	B	809	X	-	-	-
15	CLA	B	810	X	-	-	-
15	CLA	B	812	X	-	-	-
15	CLA	B	813	X	-	-	-
15	CLA	B	814	X	-	-	-
15	CLA	B	815	X	-	-	-
15	CLA	B	816	X	-	-	-
15	CLA	B	817	X	-	-	-
15	CLA	B	818	X	-	-	-
15	CLA	B	819	X	-	-	-
15	CLA	B	820	X	-	-	-
15	CLA	B	821	X	-	-	-
15	CLA	B	822	X	-	-	-
15	CLA	B	823	X	-	-	-
15	CLA	B	824	X	-	-	-
15	CLA	B	825	X	-	-	-
15	CLA	B	826	X	-	-	-
15	CLA	B	827	X	-	-	-
15	CLA	B	828	X	-	-	-
15	CLA	B	829	X	-	-	-
15	CLA	B	830	X	-	-	-
15	CLA	B	832	X	-	-	-
15	CLA	B	833	X	-	-	-
15	CLA	B	834	X	-	-	-
15	CLA	B	835	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	B	836	X	-	-	-
15	CLA	B	837	X	-	-	-
15	CLA	B	839	X	-	-	-
15	CLA	F	201	X	-	-	-
15	CLA	K	102	X	-	-	-
15	CLA	K	103	X	-	-	-
15	CLA	L	202	X	-	-	-
15	CLA	L	203	X	-	-	-
15	CLA	N	803	X	-	-	-
15	CLA	N	804	X	-	-	-
15	CLA	N	805	X	-	-	-
15	CLA	N	806	X	-	-	-
15	CLA	N	807	X	-	-	-
15	CLA	N	808	X	-	-	-
15	CLA	N	809	X	-	-	-
15	CLA	N	810	X	-	-	-
15	CLA	N	811	X	-	-	-
15	CLA	N	812	X	-	-	-
15	CLA	N	813	X	-	-	-
15	CLA	N	814	X	-	-	-
15	CLA	N	815	X	-	-	-
15	CLA	N	816	X	-	-	-
15	CLA	N	817	X	-	-	-
15	CLA	N	818	X	-	-	-
15	CLA	N	819	X	-	-	-
15	CLA	N	820	X	-	-	-
15	CLA	N	821	X	-	-	-
15	CLA	N	822	X	-	-	-
15	CLA	N	823	X	-	-	-
15	CLA	N	825	X	-	-	-
15	CLA	N	827	X	-	-	-
15	CLA	N	828	X	-	-	-
15	CLA	N	829	X	-	-	-
15	CLA	N	830	X	-	-	-
15	CLA	N	831	X	-	-	-
15	CLA	N	832	X	-	-	-
15	CLA	N	833	X	-	-	-
15	CLA	N	834	X	-	-	-
15	CLA	N	835	X	-	-	-
15	CLA	N	836	X	-	-	-
15	CLA	N	837	X	-	-	-
15	CLA	N	838	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	N	839	X	-	-	-
15	CLA	N	840	X	-	-	-
15	CLA	N	841	X	-	-	-
15	CLA	N	842	X	-	-	-
15	CLA	O	801	X	-	-	-
15	CLA	O	802	X	-	-	-
15	CLA	O	803	X	-	-	-
15	CLA	O	804	X	-	-	-
15	CLA	O	805	X	-	-	-
15	CLA	O	806	X	-	-	-
15	CLA	O	807	X	-	-	-
15	CLA	O	808	X	-	-	-
15	CLA	O	809	X	-	-	-
15	CLA	O	811	X	-	-	-
15	CLA	O	812	X	-	-	-
15	CLA	O	814	X	-	-	-
15	CLA	O	815	X	-	-	-
15	CLA	O	816	X	-	-	-
15	CLA	O	817	X	-	-	-
15	CLA	O	818	X	-	-	-
15	CLA	O	819	X	-	-	-
15	CLA	O	820	X	-	-	-
15	CLA	O	821	X	-	-	-
15	CLA	O	822	X	-	-	-
15	CLA	O	823	X	-	-	-
15	CLA	O	824	X	-	-	-
15	CLA	O	825	X	-	-	-
15	CLA	O	826	X	-	-	-
15	CLA	O	827	X	-	-	-
15	CLA	O	828	X	-	-	-
15	CLA	O	829	X	-	-	-
15	CLA	O	830	X	-	-	-
15	CLA	O	831	X	-	-	-
15	CLA	O	832	X	-	-	-
15	CLA	O	834	X	-	-	-
15	CLA	O	835	X	-	-	-
15	CLA	O	836	X	-	-	-
15	CLA	O	837	X	-	-	-
15	CLA	O	838	X	-	-	-
15	CLA	O	839	X	-	-	-
15	CLA	O	841	X	-	-	-
15	CLA	S	201	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	V	102	X	-	-	-
15	CLA	V	103	X	-	-	-
15	CLA	W	1501	X	-	-	-
15	CLA	W	1502	X	-	-	-
15	CLA	X	103	X	-	-	-
15	CLA	Z	103	X	-	-	-
15	CLA	a	803	X	-	-	-
15	CLA	a	804	X	-	-	-
15	CLA	a	805	X	-	-	-
15	CLA	a	806	X	-	-	-
15	CLA	a	807	X	-	-	-
15	CLA	a	808	X	-	-	-
15	CLA	a	809	X	-	-	-
15	CLA	a	810	X	-	-	-
15	CLA	a	811	X	-	-	-
15	CLA	a	812	X	-	-	-
15	CLA	a	813	X	-	-	-
15	CLA	a	814	X	-	-	-
15	CLA	a	815	X	-	-	-
15	CLA	a	816	X	-	-	-
15	CLA	a	817	X	-	-	-
15	CLA	a	818	X	-	-	-
15	CLA	a	819	X	-	-	-
15	CLA	a	820	X	-	-	-
15	CLA	a	821	X	-	-	-
15	CLA	a	822	X	-	-	-
15	CLA	a	823	X	-	-	-
15	CLA	a	825	X	-	-	-
15	CLA	a	827	X	-	-	-
15	CLA	a	828	X	-	-	-
15	CLA	a	829	X	-	-	-
15	CLA	a	830	X	-	-	-
15	CLA	a	831	X	-	-	-
15	CLA	a	832	X	-	-	-
15	CLA	a	833	X	-	-	-
15	CLA	a	834	X	-	-	-
15	CLA	a	835	X	-	-	-
15	CLA	a	836	X	-	-	-
15	CLA	a	837	X	-	-	-
15	CLA	a	838	X	-	-	-
15	CLA	a	839	X	-	-	-
15	CLA	a	840	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	a	841	X	-	-	-
15	CLA	a	842	X	-	-	-
15	CLA	b	801	X	-	-	-
15	CLA	b	802	X	-	-	-
15	CLA	b	803	X	-	-	-
15	CLA	b	804	X	-	-	-
15	CLA	b	805	X	-	-	-
15	CLA	b	806	X	-	-	-
15	CLA	b	807	X	-	-	-
15	CLA	b	808	X	-	-	-
15	CLA	b	809	X	-	-	-
15	CLA	b	811	X	-	-	-
15	CLA	b	812	X	-	-	-
15	CLA	b	814	X	-	-	-
15	CLA	b	815	X	-	-	-
15	CLA	b	816	X	-	-	-
15	CLA	b	817	X	-	-	-
15	CLA	b	818	X	-	-	-
15	CLA	b	819	X	-	-	-
15	CLA	b	820	X	-	-	-
15	CLA	b	821	X	-	-	-
15	CLA	b	822	X	-	-	-
15	CLA	b	823	X	-	-	-
15	CLA	b	824	X	-	-	-
15	CLA	b	825	X	-	-	-
15	CLA	b	826	X	-	-	-
15	CLA	b	827	X	-	-	-
15	CLA	b	828	X	-	-	-
15	CLA	b	829	X	-	-	-
15	CLA	b	830	X	-	-	-
15	CLA	b	831	X	-	-	-
15	CLA	b	832	X	-	-	-
15	CLA	b	834	X	-	-	-
15	CLA	b	835	X	-	-	-
15	CLA	b	836	X	-	-	-
15	CLA	b	837	X	-	-	-
15	CLA	b	838	X	-	-	-
15	CLA	b	839	X	-	-	-
15	CLA	b	841	X	-	-	-
15	CLA	f	201	X	-	-	-
15	CLA	i	102	X	-	-	-
15	CLA	i	103	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	j	202	X	-	-	-
15	CLA	j	203	X	-	-	-
15	CLA	l	103	X	-	-	-



## 2 Entry composition [i](#)

There are 24 unique types of molecules in this entry. The entry contains 75954 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	753	Total	C	N	O	S	0	0
			5900	3869	1012	988	31		
1	N	753	Total	C	N	O	S	0	0
			5900	3869	1012	988	31		
1	a	753	Total	C	N	O	S	0	0
			5900	3869	1012	988	31		

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	739	Total	C	N	O	S	0	0
			5913	3897	994	1004	18		
2	O	739	Total	C	N	O	S	0	0
			5913	3897	994	1004	18		
2	b	739	Total	C	N	O	S	0	0
			5913	3897	994	1004	18		

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			600	368	103	118	11		
3	P	80	Total	C	N	O	S	0	0
			600	368	103	118	11		
3	c	80	Total	C	N	O	S	0	0
			600	368	103	118	11		

- Molecule 4 is a protein called Photosystem I reaction center subunit II.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	139	Total	C	N	O	S	0	0
			1090	692	193	202	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	Q	139	Total	C	N	O	S	0	0
			1090	692	193	202	3		
4	d	139	Total	C	N	O	S	0	0
			1090	692	193	202	3		

- Molecule 5 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	65	Total	C	N	O		0	0
			530	341	92	97			
5	R	65	Total	C	N	O		0	0
			530	341	92	97			
5	e	65	Total	C	N	O		0	0
			530	341	92	97			

- Molecule 6 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	137	Total	C	N	O	S	0	0
			1075	698	176	197	4		
6	S	137	Total	C	N	O	S	0	0
			1075	698	176	197	4		
6	f	137	Total	C	N	O	S	0	0
			1075	698	176	197	4		

- Molecule 7 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	42	Total	C	N	O	S	0	0
			351	247	47	55	2		
7	T	42	Total	C	N	O	S	0	0
			351	247	47	55	2		
7	g	42	Total	C	N	O	S	0	0
			351	247	47	55	2		

- Molecule 8 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	46	Total	C	N	O	S	0	0
			373	256	54	59	4		
8	U	46	Total	C	N	O	S	0	0
			373	256	54	59	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	46	Total	C	N	O	S	0	0
			373	256	54	59	4		

- Molecule 9 is a protein called Photosystem I reaction center subunit Psak.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	75	Total	C	N	O	S	0	0
			539	356	88	94	1		
9	V	75	Total	C	N	O	S	0	0
			539	356	88	94	1		
9	i	75	Total	C	N	O	S	0	0
			539	356	88	94	1		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	12	MET	-	initiating methionine	UNP K9TX25
V	12	MET	-	initiating methionine	UNP K9TX25
i	12	MET	-	initiating methionine	UNP K9TX25

- Molecule 10 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	172	Total	C	N	O	S	0	0
			1309	839	224	242	4		
10	W	172	Total	C	N	O	S	0	0
			1309	839	224	242	4		
10	j	172	Total	C	N	O	S	0	0
			1309	839	224	242	4		

- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	31	Total	C	N	O	S	0	0
			240	160	37	42	1		
11	Y	31	Total	C	N	O	S	0	0
			240	160	37	42	1		
11	k	31	Total	C	N	O	S	0	0
			240	160	37	42	1		

There are 3 discrepancies between the modelled and reference sequences:

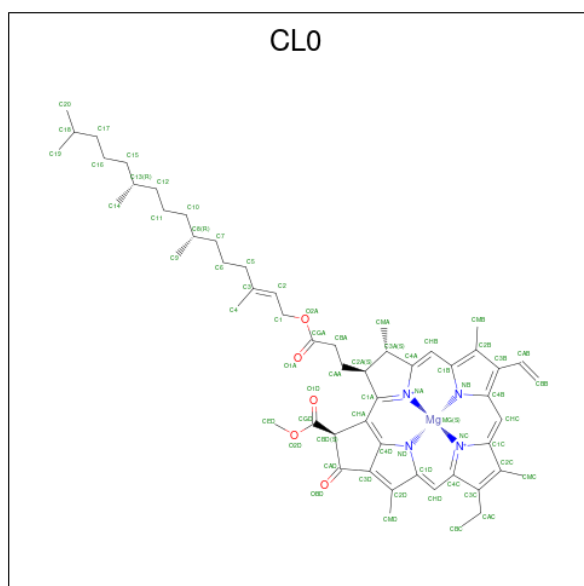


Chain	Residue	Modelled	Actual	Comment	Reference
M	0	MET	-	initiating methionine	UNP K9TSY6
Y	0	MET	-	initiating methionine	UNP K9TSY6
k	0	MET	-	initiating methionine	UNP K9TSY6

- Molecule 12 is a protein called Photosystem one Psax.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	X	29	Total	C	N	O	0	0
			227	157	36	34		
12	Z	29	Total	C	N	O	0	0
			227	157	36	34		
12	l	29	Total	C	N	O	0	0
			227	157	36	34		

- Molecule 13 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula:  $C_{55}H_{72}MgN_4O_5$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
13	A	1	Total	C	Mg	N	O
			65	55	1	4	5
13	N	1	Total	C	Mg	N	O
			65	55	1	4	5
13	a	1	Total	C	Mg	N	O
			65	55	1	4	5

- Molecule 14 is Chlorophyll F (CCD ID: F6C) (formula:  $C_{55}H_{68}MgN_4O_6$ ) (labeled as "Ligand of Interest" by depositor).





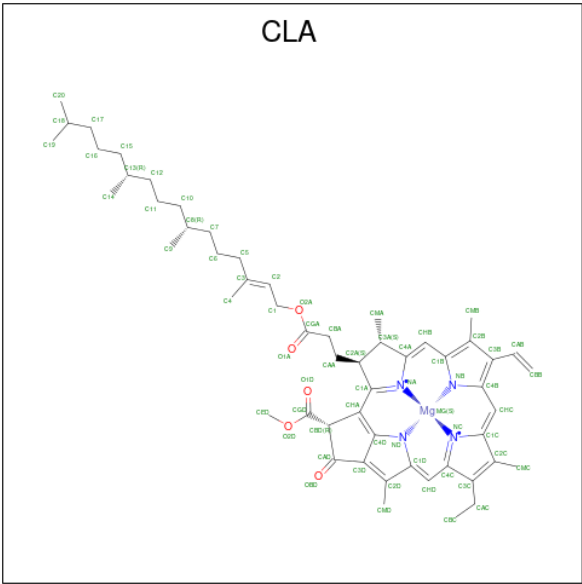
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Mol	Chain	Residues	Atoms					AltConf
14	O	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
14	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
14	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
14	a	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
14	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
14	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
14	b	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
14	b	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
14	b	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
14	j	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 15 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
15	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	A	1	Total 57	C 47	Mg 1	N 4	O 5	0
15	A	1	Total 57	C 47	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 56	C 46	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
15	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
15	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	B	1	Total 57	C 47	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	B	1	Total 53	C 43	Mg 1	N 4	O 5	0
15	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 62	C 52	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	K	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	L	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	X	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	N	1	Total 57	C 47	Mg 1	N 4	O 5	0
15	N	1	Total 57	C 47	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 54	C 44	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 56	C 46	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	N	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 54	C 44	Mg 1	N 4	O 5	0
15	N	1	Total 51	C 41	Mg 1	N 4	O 5	0
15	N	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	O	1	Total 56	C 46	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	O	1	Total 57	C 47	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	O	1	Total 53	C 43	Mg 1	N 4	O 5	0
15	O	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 62	C 52	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	V	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	V	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	W	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	W	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	Z	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	a	1	Total 57	C 47	Mg 1	N 4	O 5	0
15	a	1	Total 57	C 47	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 54	C 44	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 56	C 46	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 54	C 44	Mg 1	N 4	O 5	0
15	a	1	Total 51	C 41	Mg 1	N 4	O 5	0
15	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b	1	Total 56	C 46	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b	1	Total 57	C 47	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b	1	Total 53	C 43	Mg 1	N 4	O 5	0
15	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 62	C 52	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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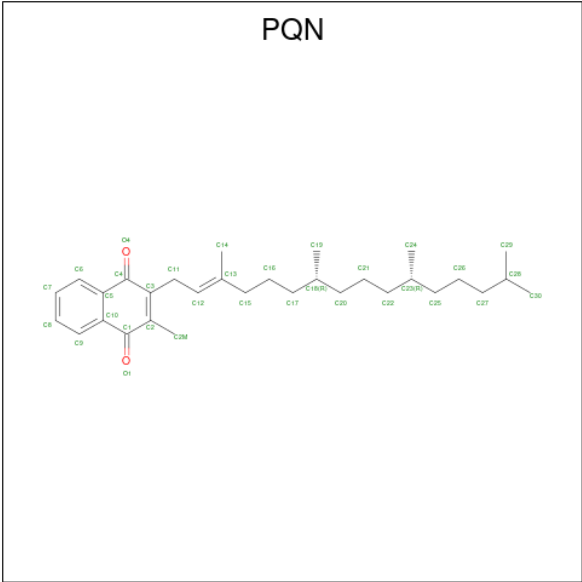


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Mol	Chain	Residues	Atoms					AltConf
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	i	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	i	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	j	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	j	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	l	1	Total 55	C 45	Mg 1	N 4	O 5	0

- Molecule 16 is PHYLLOQUINONE (CCD ID: PQN) (formula:  $C_{31}H_{46}O_2$ ).

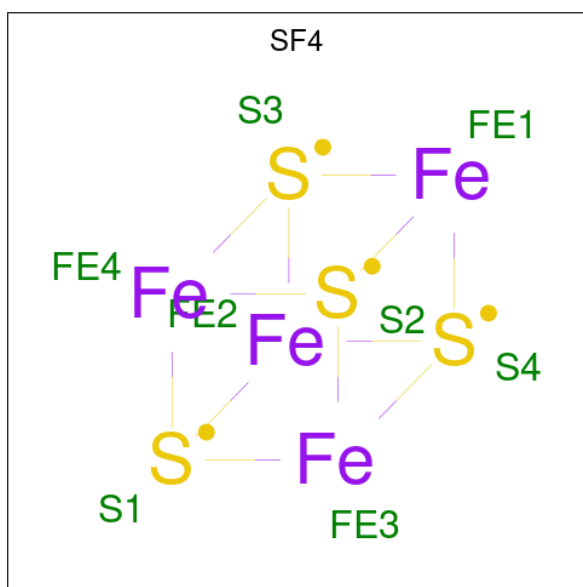




Mol	Chain	Residues	Atoms			AltConf
16	A	1	Total	C	O	0
			33	31	2	
16	B	1	Total	C	O	0
			33	31	2	
16	N	1	Total	C	O	0
			33	31	2	
16	O	1	Total	C	O	0
			33	31	2	
16	a	1	Total	C	O	0
			33	31	2	
16	b	1	Total	C	O	0
			33	31	2	

- Molecule 17 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).

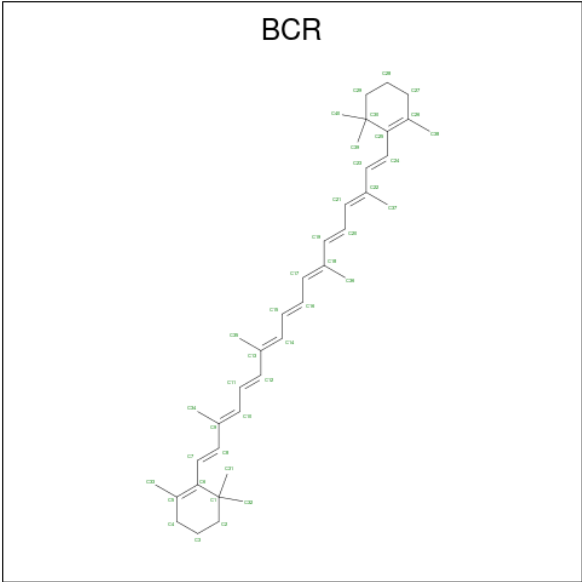




Mol	Chain	Residues	Atoms			AltConf
17	A	1	Total	Fe	S	0
			8	4	4	
17	C	1	Total	Fe	S	0
			8	4	4	
17	C	1	Total	Fe	S	0
			8	4	4	
17	N	1	Total	Fe	S	0
			8	4	4	
17	P	1	Total	Fe	S	0
			8	4	4	
17	P	1	Total	Fe	S	0
			8	4	4	
17	a	1	Total	Fe	S	0
			8	4	4	
17	c	1	Total	Fe	S	0
			8	4	4	
17	c	1	Total	Fe	S	0
			8	4	4	

- Molecule 18 is BETA-CAROTENE (CCD ID: BCR) (formula:  $C_{40}H_{56}$ ).





Mol	Chain	Residues	Atoms		AltConf
18	A	1	Total	C	0
			40	40	
18	A	1	Total	C	0
			40	40	
18	A	1	Total	C	0
			40	40	
18	A	1	Total	C	0
			40	40	
18	A	1	Total	C	0
			40	40	
18	A	1	Total	C	0
			40	40	
18	B	1	Total	C	0
			40	40	
18	B	1	Total	C	0
			40	40	
18	B	1	Total	C	0
			40	40	
18	B	1	Total	C	0
			40	40	
18	B	1	Total	C	0
			40	40	
18	F	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
18	F	1	Total C 40 40	0
18	I	1	Total C 40 40	0
18	I	1	Total C 40 40	0
18	J	1	Total C 40 40	0
18	K	1	Total C 25 25	0
18	L	1	Total C 40 40	0
18	L	1	Total C 40 40	0
18	M	1	Total C 40 40	0
18	N	1	Total C 40 40	0
18	N	1	Total C 40 40	0
18	N	1	Total C 40 40	0
18	N	1	Total C 40 40	0
18	N	1	Total C 40 40	0
18	N	1	Total C 40 40	0
18	N	1	Total C 40 40	0
18	N	1	Total C 40 40	0
18	O	1	Total C 40 40	0
18	O	1	Total C 40 40	0
18	O	1	Total C 40 40	0
18	O	1	Total C 40 40	0
18	O	1	Total C 40 40	0
18	O	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
18	O	1	Total C 40 40	0
18	S	1	Total C 40 40	0
18	T	1	Total C 40 40	0
18	T	1	Total C 40 40	0
18	U	1	Total C 40 40	0
18	V	1	Total C 25 25	0
18	W	1	Total C 40 40	0
18	W	1	Total C 40 40	0
18	Y	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	b	1	Total C 40 40	0
18	b	1	Total C 40 40	0
18	b	1	Total C 40 40	0
18	b	1	Total C 40 40	0
18	b	1	Total C 40 40	0

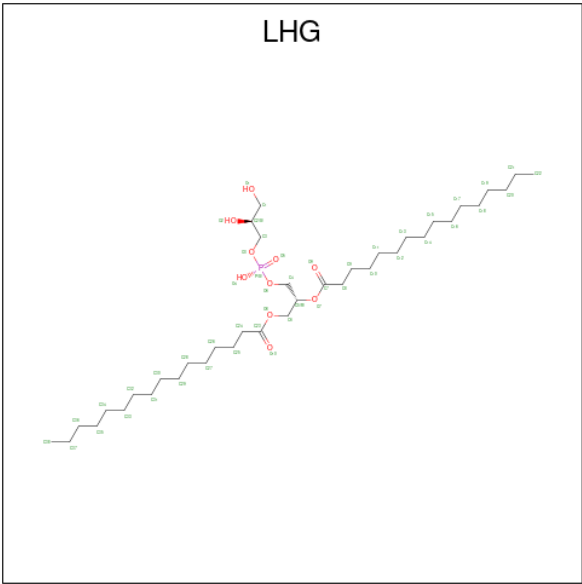
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Mol	Chain	Residues	Atoms		AltConf
18	b	1	Total	C	0
			40	40	
18	f	1	Total	C	0
			40	40	
18	f	1	Total	C	0
			40	40	
18	g	1	Total	C	0
			40	40	
18	g	1	Total	C	0
			40	40	
18	h	1	Total	C	0
			40	40	
18	i	1	Total	C	0
			25	25	
18	j	1	Total	C	0
			40	40	
18	j	1	Total	C	0
			40	40	
18	k	1	Total	C	0
			40	40	

- Molecule 19 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



Mol	Chain	Residues	Atoms				AltConf
19	A	1	Total	C	O	P	0
			42	31	10	1	

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Mol	Chain	Residues	Atoms				AltConf
19	L	1	Total 49	C 38	O 10	P 1	0
19	M	1	Total 49	C 38	O 10	P 1	0
19	X	1	Total 44	C 33	O 10	P 1	0
19	X	1	Total 49	C 38	O 10	P 1	0
19	N	1	Total 42	C 31	O 10	P 1	0
19	W	1	Total 49	C 38	O 10	P 1	0
19	Y	1	Total 49	C 38	O 10	P 1	0
19	Z	1	Total 44	C 33	O 10	P 1	0
19	Z	1	Total 49	C 38	O 10	P 1	0
19	a	1	Total 42	C 31	O 10	P 1	0
19	j	1	Total 49	C 38	O 10	P 1	0
19	k	1	Total 49	C 38	O 10	P 1	0
19	l	1	Total 44	C 33	O 10	P 1	0
19	l	1	Total 49	C 38	O 10	P 1	0

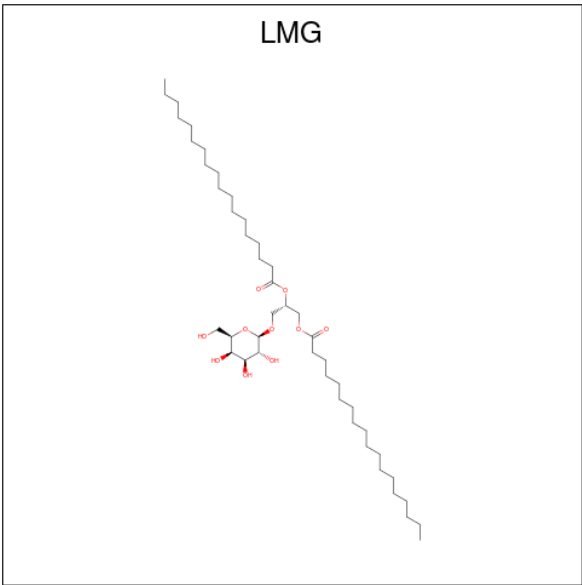
- Molecule 20 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).





- Molecule 21 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).





Mol	Chain	Residues	Atoms			AltConf
21	A	1	Total	C	O	0
			44	34	10	
21	B	1	Total	C	O	0
			55	45	10	
21	I	1	Total	C	O	0
			37	27	10	
21	J	1	Total	C	O	0
			55	45	10	
21	L	1	Total	C	O	0
			50	40	10	
21	N	1	Total	C	O	0
			44	34	10	
21	O	1	Total	C	O	0
			55	45	10	
21	T	1	Total	C	O	0
			37	27	10	
21	U	1	Total	C	O	0
			55	45	10	
21	W	1	Total	C	O	0
			50	40	10	
21	a	1	Total	C	O	0
			44	34	10	
21	b	1	Total	C	O	0
			55	45	10	
21	g	1	Total	C	O	0
			37	27	10	
21	h	1	Total	C	O	0
			55	45	10	

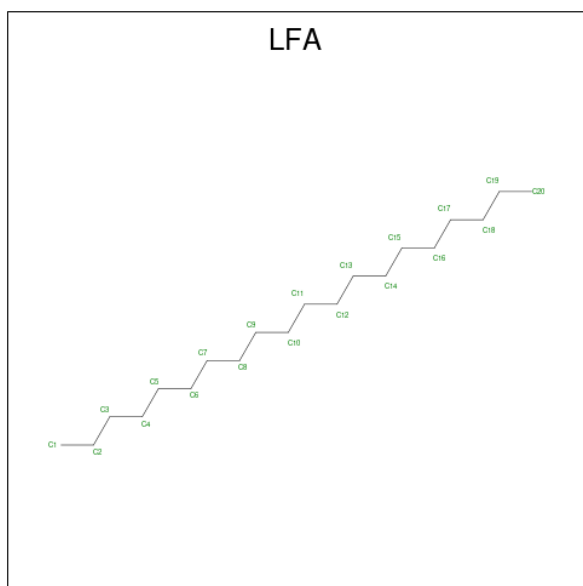
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Mol	Chain	Residues	Atoms			AltConf
21	j	1	Total	C	O	0
			50	40	10	

- Molecule 22 is EICOSANE (CCD ID: LFA) (formula:  $C_{20}H_{42}$ ).



Mol	Chain	Residues	Atoms		AltConf
22	B	1	Total	C	0
			16	16	
22	L	1	Total	C	0
			15	15	
22	O	1	Total	C	0
			16	16	
22	W	1	Total	C	0
			15	15	
22	f	1	Total	C	0
			16	16	
22	j	1	Total	C	0
			15	15	

- Molecule 23 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
23	L	1	Total	Ca	0
			1	1	
23	W	1	Total	Ca	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
23	j	1	Total 1	Ca 1	0

- Molecule 24 is water.

Mol	Chain	Residues	Atoms		AltConf
24	A	50	Total 50	O 50	0
24	B	55	Total 55	O 55	0
24	C	3	Total 3	O 3	0
24	D	11	Total 11	O 11	0
24	E	2	Total 2	O 2	0
24	F	2	Total 2	O 2	0
24	I	2	Total 2	O 2	0
24	K	1	Total 1	O 1	0
24	L	8	Total 8	O 8	0
24	N	51	Total 51	O 51	0
24	O	55	Total 55	O 55	0
24	P	2	Total 2	O 2	0
24	Q	11	Total 11	O 11	0
24	R	2	Total 2	O 2	0
24	S	2	Total 2	O 2	0
24	T	2	Total 2	O 2	0
24	V	1	Total 1	O 1	0
24	W	9	Total 9	O 9	0

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Mol	Chain	Residues	Atoms		AltConf
24	a	52	Total 52	O 52	0
24	b	55	Total 55	O 55	0
24	c	3	Total 3	O 3	0
24	d	10	Total 10	O 10	0
24	e	2	Total 2	O 2	0
24	f	2	Total 2	O 2	0
24	g	3	Total 3	O 3	0
24	i	1	Total 1	O 1	0
24	j	8	Total 8	O 8	0

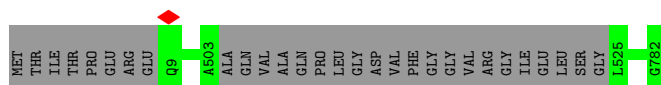


### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

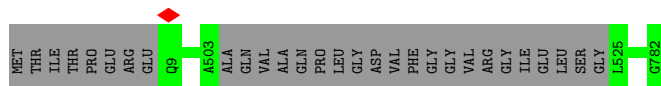
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain A:  96%



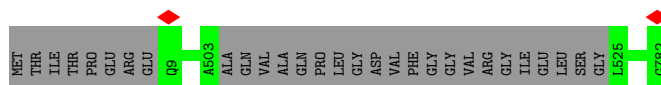
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain N:  96%



- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain a:  96%



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:  100%



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain O:  100%





- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain b:  100%



- Molecule 3: Photosystem I iron-sulfur center

Chain C:  99%



- Molecule 3: Photosystem I iron-sulfur center

Chain P:  99%



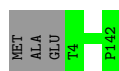
- Molecule 3: Photosystem I iron-sulfur center

Chain c:  99%



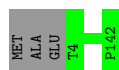
- Molecule 4: Photosystem I reaction center subunit II

Chain D:  98%



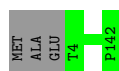
- Molecule 4: Photosystem I reaction center subunit II

Chain Q:  98%



- Molecule 4: Photosystem I reaction center subunit II

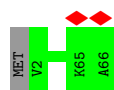
Chain d:  98%





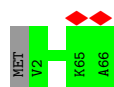
- Molecule 5: Photosystem I reaction center subunit IV

Chain E:  98%



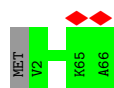
- Molecule 5: Photosystem I reaction center subunit IV

Chain R:  98%




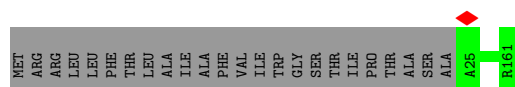
- Molecule 5: Photosystem I reaction center subunit IV

Chain e:  98%




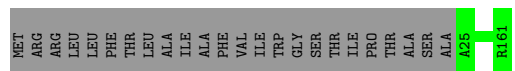
- Molecule 6: Photosystem I reaction center subunit III

Chain F:  85% 15%




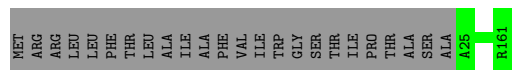
- Molecule 6: Photosystem I reaction center subunit III

Chain S:  85% 15%




- Molecule 6: Photosystem I reaction center subunit III

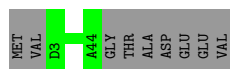
Chain f:  85% 15%



- Molecule 7: Photosystem I reaction center subunit VIII

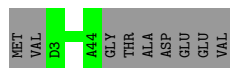
Chain I:  82% 18%





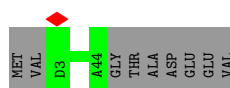
- Molecule 7: Photosystem I reaction center subunit VIII

Chain T: 82% 18%



- Molecule 7: Photosystem I reaction center subunit VIII

Chain g: 82% 18%



- Molecule 8: Photosystem I reaction center subunit IX

Chain J: 100%

There are no outlier residues recorded for this chain.

- Molecule 8: Photosystem I reaction center subunit IX

Chain U: 100%

There are no outlier residues recorded for this chain.

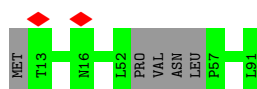
- Molecule 8: Photosystem I reaction center subunit IX

Chain h: 100%

There are no outlier residues recorded for this chain.

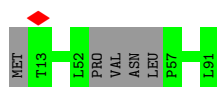
- Molecule 9: Photosystem I reaction center subunit PsaK

Chain K: 94% 6%



- Molecule 9: Photosystem I reaction center subunit PsaK

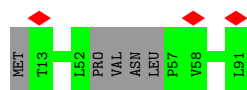
Chain V: 94% 6%





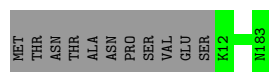
- Molecule 9: Photosystem I reaction center subunit PsaK

Chain i:  94% 6%



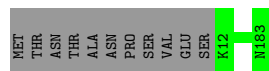
- Molecule 10: Photosystem I reaction center subunit XI

Chain L:  94% 6%



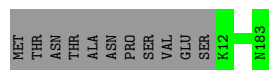
- Molecule 10: Photosystem I reaction center subunit XI

Chain W:  94% 6%



- Molecule 10: Photosystem I reaction center subunit XI

Chain j:  94% 6%



- Molecule 11: Photosystem I reaction center subunit XII

Chain M:  97% .



- Molecule 11: Photosystem I reaction center subunit XII

Chain Y:  97% .



- Molecule 11: Photosystem I reaction center subunit XII

Chain k:  97% .





- Molecule 12: Photosystem one PsaX

Chain X:  100%

There are no outlier residues recorded for this chain.

- Molecule 12: Photosystem one PsaX

Chain Z:  100%



- Molecule 12: Photosystem one PsaX

Chain I:  100%





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	83138	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.504	Depositor
Minimum map value	-0.162	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.054	Depositor
Map size (Å)	552.6, 552.6, 552.6	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.92099994, 0.92099994, 0.92099994	Depositor



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PQN, BCR, CL0, CLA, SF4, LHG, F6C, LFA, CA, LMG, LMT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.26	0/6106	0.44	0/8323
1	N	0.25	0/6106	0.43	0/8323
1	a	0.25	0/6106	0.43	0/8323
2	B	0.26	0/6139	0.44	0/8394
2	O	0.25	0/6139	0.42	0/8394
2	b	0.25	0/6139	0.42	0/8394
3	C	0.26	0/610	0.52	0/827
3	P	0.25	0/610	0.51	0/827
3	c	0.26	0/610	0.52	0/827
4	D	0.26	0/1115	0.50	0/1501
4	Q	0.26	0/1115	0.49	0/1501
4	d	0.26	0/1115	0.49	0/1501
5	E	0.26	0/540	0.49	0/728
5	R	0.26	0/540	0.48	0/728
5	e	0.26	0/540	0.48	0/728
6	F	0.26	0/1104	0.49	0/1501
6	S	0.25	0/1104	0.48	0/1501
6	f	0.25	0/1104	0.48	0/1501
7	I	0.27	0/366	0.46	0/503
7	T	0.26	0/366	0.45	0/503
7	g	0.26	0/366	0.44	0/503
8	J	0.26	0/386	0.37	0/526
8	U	0.25	0/386	0.38	0/526
8	h	0.25	0/386	0.36	0/526
9	K	0.24	0/550	0.46	0/751
9	V	0.23	0/550	0.45	0/751
9	i	0.23	0/550	0.44	0/751
10	L	0.26	0/1340	0.48	0/1821
10	W	0.25	0/1340	0.47	0/1821
10	j	0.26	0/1340	0.47	0/1821
11	M	0.24	0/243	0.42	0/329
11	Y	0.24	0/243	0.40	0/329



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
11	k	0.24	0/243	0.40	0/329
12	X	0.25	0/233	0.40	0/319
12	Z	0.24	0/233	0.39	0/319
12	l	0.24	0/233	0.39	0/319
All	All	0.25	0/56196	0.44	0/76569

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	749/782 (96%)	730 (98%)	19 (2%)	0	100	100
1	N	749/782 (96%)	736 (98%)	13 (2%)	0	100	100
1	a	749/782 (96%)	735 (98%)	14 (2%)	0	100	100
2	B	737/740 (100%)	723 (98%)	14 (2%)	0	100	100
2	O	737/740 (100%)	723 (98%)	14 (2%)	0	100	100
2	b	737/740 (100%)	723 (98%)	14 (2%)	0	100	100
3	C	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
3	P	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
3	c	78/81 (96%)	76 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	137/142 (96%)	135 (98%)	2 (2%)	0	100	100
4	Q	137/142 (96%)	134 (98%)	3 (2%)	0	100	100
4	d	137/142 (96%)	136 (99%)	1 (1%)	0	100	100
5	E	63/66 (96%)	63 (100%)	0	0	100	100
5	R	63/66 (96%)	63 (100%)	0	0	100	100
5	e	63/66 (96%)	63 (100%)	0	0	100	100
6	F	135/161 (84%)	132 (98%)	3 (2%)	0	100	100
6	S	135/161 (84%)	131 (97%)	4 (3%)	0	100	100
6	f	135/161 (84%)	131 (97%)	4 (3%)	0	100	100
7	I	40/51 (78%)	38 (95%)	2 (5%)	0	100	100
7	T	40/51 (78%)	38 (95%)	2 (5%)	0	100	100
7	g	40/51 (78%)	38 (95%)	2 (5%)	0	100	100
8	J	44/46 (96%)	44 (100%)	0	0	100	100
8	U	44/46 (96%)	44 (100%)	0	0	100	100
8	h	44/46 (96%)	44 (100%)	0	0	100	100
9	K	71/80 (89%)	70 (99%)	1 (1%)	0	100	100
9	V	71/80 (89%)	70 (99%)	1 (1%)	0	100	100
9	i	71/80 (89%)	70 (99%)	1 (1%)	0	100	100
10	L	170/183 (93%)	170 (100%)	0	0	100	100
10	W	170/183 (93%)	170 (100%)	0	0	100	100
10	j	170/183 (93%)	170 (100%)	0	0	100	100
11	M	29/32 (91%)	29 (100%)	0	0	100	100
11	Y	29/32 (91%)	29 (100%)	0	0	100	100
11	k	29/32 (91%)	29 (100%)	0	0	100	100
12	X	27/29 (93%)	25 (93%)	2 (7%)	0	100	100
12	Z	27/29 (93%)	25 (93%)	2 (7%)	0	100	100
12	l	27/29 (93%)	25 (93%)	2 (7%)	0	100	100
All	All	6840/7179 (95%)	6715 (98%)	125 (2%)	0	100	100

There are no Ramachandran outliers to report.



### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	600/623 (96%)	600 (100%)	0	100	100
1	N	600/623 (96%)	600 (100%)	0	100	100
1	a	600/623 (96%)	600 (100%)	0	100	100
2	B	594/595 (100%)	594 (100%)	0	100	100
2	O	594/595 (100%)	594 (100%)	0	100	100
2	b	594/595 (100%)	594 (100%)	0	100	100
3	C	68/69 (99%)	68 (100%)	0	100	100
3	P	68/69 (99%)	68 (100%)	0	100	100
3	c	68/69 (99%)	68 (100%)	0	100	100
4	D	114/116 (98%)	114 (100%)	0	100	100
4	Q	114/116 (98%)	114 (100%)	0	100	100
4	d	114/116 (98%)	114 (100%)	0	100	100
5	E	57/58 (98%)	57 (100%)	0	100	100
5	R	57/58 (98%)	57 (100%)	0	100	100
5	e	57/58 (98%)	57 (100%)	0	100	100
6	F	116/135 (86%)	116 (100%)	0	100	100
6	S	116/135 (86%)	116 (100%)	0	100	100
6	f	116/135 (86%)	116 (100%)	0	100	100
7	I	37/44 (84%)	37 (100%)	0	100	100
7	T	37/44 (84%)	37 (100%)	0	100	100
7	g	37/44 (84%)	37 (100%)	0	100	100
8	J	41/41 (100%)	41 (100%)	0	100	100
8	U	41/41 (100%)	41 (100%)	0	100	100
8	h	41/41 (100%)	41 (100%)	0	100	100
9	K	60/65 (92%)	60 (100%)	0	100	100
9	V	60/65 (92%)	60 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	i	60/65 (92%)	60 (100%)	0	100	100
10	L	135/146 (92%)	135 (100%)	0	100	100
10	W	135/146 (92%)	135 (100%)	0	100	100
10	j	135/146 (92%)	135 (100%)	0	100	100
11	M	26/27 (96%)	26 (100%)	0	100	100
11	Y	26/27 (96%)	26 (100%)	0	100	100
11	k	26/27 (96%)	26 (100%)	0	100	100
12	X	24/24 (100%)	24 (100%)	0	100	100
12	Z	24/24 (100%)	24 (100%)	0	100	100
12	l	24/24 (100%)	24 (100%)	0	100	100
All	All	5616/5829 (96%)	5616 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
6	S	52	ASN
5	e	19	GLN
1	a	153	ASN
6	f	52	ASN
4	d	53	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.



## 5.6 Ligand geometry

Of 402 ligands modelled in this entry, 3 are monoatomic - leaving 399 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	CLA	a	822	24	65,73,73	1.49	6 (9%)	76,113,113	1.36	7 (9%)
18	BCR	O	844	-	41,41,41	0.31	0	56,56,56	0.67	0
20	LMT	N	852	-	32,32,36	0.57	0	43,43,47	0.67	0
18	BCR	F	202	-	41,41,41	0.32	0	56,56,56	1.00	4 (7%)
15	CLA	O	826	2	65,73,73	1.47	6 (9%)	76,113,113	1.42	7 (9%)
15	CLA	O	814	2	65,73,73	1.49	6 (9%)	76,113,113	1.37	8 (10%)
22	LFA	B	848	-	15,15,19	0.23	0	14,14,18	0.20	0
15	CLA	N	828	1	65,73,73	1.47	7 (10%)	76,113,113	1.38	6 (7%)
15	CLA	b	817	2	65,73,73	1.52	6 (9%)	76,113,113	1.35	8 (10%)
15	CLA	a	825	1	65,73,73	1.48	6 (9%)	76,113,113	1.34	8 (10%)
15	CLA	a	817	24	45,53,73	1.81	5 (11%)	52,89,113	1.58	6 (11%)
15	CLA	b	816	2	57,65,73	1.56	5 (8%)	66,103,113	1.47	7 (10%)
15	CLA	A	806	1	65,73,73	1.45	6 (9%)	76,113,113	1.40	7 (9%)
15	CLA	O	835	24	45,53,73	1.77	6 (13%)	52,89,113	1.62	6 (11%)
15	CLA	a	809	1	60,68,73	1.53	5 (8%)	70,107,113	1.40	8 (11%)
15	CLA	b	839	2	65,73,73	1.47	6 (9%)	76,113,113	1.42	7 (9%)
15	CLA	b	805	2	65,73,73	1.46	6 (9%)	76,113,113	1.43	7 (9%)
20	LMT	A	854	-	36,36,36	0.55	0	47,47,47	0.62	0
15	CLA	N	841	1	65,73,73	1.47	6 (9%)	76,113,113	1.38	7 (9%)
21	LMG	b	849	-	55,55,55	0.49	0	63,63,63	0.60	0
15	CLA	K	102	9	45,53,73	1.78	6 (13%)	52,89,113	1.57	6 (11%)
18	BCR	M	101	-	41,41,41	0.32	0	56,56,56	0.67	1 (1%)
15	CLA	O	815	2	45,53,73	1.77	5 (11%)	52,89,113	1.65	8 (15%)
15	CLA	W	1502	10	60,68,73	1.54	5 (8%)	70,107,113	1.41	10 (14%)
15	CLA	b	823	2	55,63,73	1.63	7 (12%)	64,101,113	1.37	8 (12%)
15	CLA	O	830	2	65,73,73	1.48	6 (9%)	76,113,113	1.36	7 (9%)
15	CLA	a	840	1	50,58,73	1.68	5 (10%)	58,95,113	1.56	8 (13%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	CLA	b	827	2	62,70,73	1.51	7 (11%)	72,109,113	1.39	7 (9%)
18	BCR	A	849	-	41,41,41	0.32	0	56,56,56	0.61	0
21	LMG	I	103	-	37,37,55	0.56	0	45,45,63	0.66	0
15	CLA	A	832	1	50,58,73	1.67	6 (12%)	58,95,113	1.54	7 (12%)
15	CLA	N	821	1	60,68,73	1.54	6 (10%)	70,107,113	1.40	7 (10%)
18	BCR	T	102	-	41,41,41	0.29	0	56,56,56	0.48	0
15	CLA	A	835	1	65,73,73	1.47	6 (9%)	76,113,113	1.38	8 (10%)
15	CLA	V	103	24	50,58,73	1.71	5 (10%)	58,95,113	1.54	9 (15%)
18	BCR	I	102	-	41,41,41	0.29	0	56,56,56	0.47	0
18	BCR	A	850	-	41,41,41	0.33	0	56,56,56	0.86	0
15	CLA	a	810	1	57,65,73	1.56	6 (10%)	66,103,113	1.52	7 (10%)
15	CLA	b	808	2	65,73,73	1.45	6 (9%)	76,113,113	1.43	9 (11%)
18	BCR	b	848	-	41,41,41	0.30	0	56,56,56	0.63	0
15	CLA	N	823	1	56,64,73	1.59	5 (8%)	65,102,113	1.48	7 (10%)
18	BCR	a	845	-	41,41,41	0.36	0	56,56,56	0.93	0
15	CLA	O	811	2	65,73,73	1.48	5 (7%)	76,113,113	1.36	8 (10%)
18	BCR	A	847	-	41,41,41	0.31	0	56,56,56	0.61	1 (1%)
15	CLA	a	804	1	65,73,73	1.51	6 (9%)	76,113,113	1.37	8 (10%)
15	CLA	B	810	2	45,53,73	1.79	5 (11%)	52,89,113	1.56	7 (13%)
15	CLA	b	813	2	56,64,73	1.59	6 (10%)	65,102,113	1.49	8 (12%)
18	BCR	b	847	-	41,41,41	0.32	0	56,56,56	0.87	2 (3%)
14	F6C	N	824	24	55,60,74	2.01	13 (23%)	53,97,114	2.45	15 (28%)
15	CLA	N	817	24	45,53,73	1.81	5 (11%)	52,89,113	1.59	6 (11%)
15	CLA	b	831	2	65,73,73	1.47	6 (9%)	76,113,113	1.37	9 (11%)
15	CLA	O	809	2	65,73,73	1.48	6 (9%)	76,113,113	1.37	8 (10%)
15	CLA	O	818	2	60,68,73	1.54	5 (8%)	70,107,113	1.38	7 (10%)
15	CLA	O	834	2	55,63,73	1.60	6 (10%)	64,101,113	1.47	7 (10%)
15	CLA	N	814	1	65,73,73	1.46	6 (9%)	76,113,113	1.39	7 (9%)
15	CLA	a	827	24	55,63,73	1.60	5 (9%)	64,101,113	1.52	9 (14%)
16	PQN	O	842	-	34,34,34	0.35	0	42,45,45	0.59	1 (2%)
21	LMG	A	855	-	44,44,55	0.53	0	52,52,63	0.63	0
15	CLA	a	820	1	65,73,73	1.45	5 (7%)	76,113,113	1.51	10 (13%)
15	CLA	A	823	1	56,64,73	1.59	5 (8%)	65,102,113	1.48	7 (10%)
18	BCR	N	848	-	41,41,41	0.31	0	56,56,56	0.55	0
18	BCR	B	845	-	41,41,41	0.32	0	56,56,56	0.87	2 (3%)
15	CLA	B	821	2	55,63,73	1.63	7 (12%)	64,101,113	1.36	8 (12%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	CLA	N	838	1	55,63,73	1.58	6 (10%)	64,101,113	1.47	7 (10%)
15	CLA	B	804	2	65,73,73	1.46	6 (9%)	76,113,113	1.42	7 (9%)
18	BCR	F	203	-	41,41,41	0.30	0	56,56,56	0.50	0
17	SF4	A	844	1,2	0,12,12	-	-	-	-	-
15	CLA	i	102	9	45,53,73	1.78	6 (13%)	52,89,113	1.57	6 (11%)
16	PQN	b	842	-	34,34,34	0.35	0	42,45,45	0.59	1 (2%)
15	CLA	N	813	1	54,62,73	1.61	5 (9%)	62,99,113	1.51	8 (12%)
15	CLA	B	808	2	65,73,73	1.47	6 (9%)	76,113,113	1.36	8 (10%)
15	CLA	B	805	2	65,73,73	1.45	6 (9%)	76,113,113	1.42	7 (9%)
15	CLA	O	805	2	65,73,73	1.46	6 (9%)	76,113,113	1.42	7 (9%)
22	LFA	W	1507	-	14,14,19	0.24	0	13,13,18	0.23	0
15	CLA	A	808	1	45,53,73	1.75	6 (13%)	52,89,113	1.64	8 (15%)
15	CLA	B	827	2	65,73,73	1.47	5 (7%)	76,113,113	1.43	8 (10%)
18	BCR	N	857	-	41,41,41	0.42	0	56,56,56	1.31	8 (14%)
15	CLA	A	811	1	57,65,73	1.56	6 (10%)	66,103,113	1.45	7 (10%)
14	F6C	N	826	24	69,74,74	1.81	12 (17%)	70,114,114	2.23	19 (27%)
15	CLA	A	813	1	54,62,73	1.61	5 (9%)	62,99,113	1.52	9 (14%)
15	CLA	a	832	1	50,58,73	1.67	6 (12%)	58,95,113	1.54	8 (13%)
19	LHG	Z	101	-	43,43,48	0.54	0	46,49,54	0.51	0
18	BCR	L	205	-	41,41,41	0.35	0	56,56,56	0.66	0
18	BCR	f	202	-	41,41,41	0.32	0	56,56,56	0.99	3 (5%)
15	CLA	a	837	1	51,59,73	1.67	5 (9%)	59,96,113	1.52	9 (15%)
15	CLA	B	801	2	65,73,73	1.47	6 (9%)	76,113,113	1.32	8 (10%)
18	BCR	A	845	-	41,41,41	0.35	0	56,56,56	0.95	1 (1%)
15	CLA	O	801	2	65,73,73	1.47	7 (10%)	76,113,113	1.31	8 (10%)
18	BCR	b	844	-	41,41,41	0.31	0	56,56,56	0.63	0
15	CLA	O	839	2	65,73,73	1.47	6 (9%)	76,113,113	1.41	8 (10%)
15	CLA	N	842	1	65,73,73	1.51	6 (9%)	76,113,113	1.34	8 (10%)
15	CLA	a	815	1	55,63,73	1.61	6 (10%)	64,101,113	1.49	8 (12%)
15	CLA	A	816	1	45,53,73	1.80	5 (11%)	52,89,113	1.57	7 (13%)
15	CLA	A	834	1	65,73,73	1.49	6 (9%)	76,113,113	1.33	7 (9%)
15	CLA	B	817	24	65,73,73	1.50	5 (7%)	76,113,113	1.35	8 (10%)
15	CLA	B	828	2	65,73,73	1.48	6 (9%)	76,113,113	1.34	6 (7%)
15	CLA	b	802	24	65,73,73	1.48	5 (7%)	76,113,113	1.38	7 (9%)
15	CLA	b	822	24	53,61,73	1.63	6 (11%)	61,98,113	1.55	7 (11%)
15	CLA	B	833	24	45,53,73	1.77	6 (13%)	52,89,113	1.62	6 (11%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	LMT	A	853	-	29,29,36	0.57	0	40,40,47	1.42	5 (12%)
15	CLA	a	828	1	65,73,73	1.47	7 (10%)	76,113,113	1.39	6 (7%)
18	BCR	a	846	-	41,41,41	0.32	0	56,56,56	0.67	1 (1%)
14	F6C	a	826	24	69,74,74	1.79	12 (17%)	70,114,114	2.24	18 (25%)
17	SF4	P	102	3	0,12,12	-	-	-		
17	SF4	C	102	3	0,12,12	-	-	-		
15	CLA	V	102	9	45,53,73	1.78	6 (13%)	52,89,113	1.57	6 (11%)
15	CLA	b	829	2	65,73,73	1.47	5 (7%)	76,113,113	1.44	8 (10%)
15	CLA	N	819	1	65,73,73	1.50	7 (10%)	76,113,113	1.34	9 (11%)
15	CLA	a	838	1	55,63,73	1.58	6 (10%)	64,101,113	1.47	7 (10%)
15	CLA	A	829	1	60,68,73	1.53	6 (10%)	70,107,113	1.42	7 (10%)
14	F6C	B	831	2	69,74,74	1.78	13 (18%)	70,114,114	2.24	16 (22%)
15	CLA	b	821	2	45,53,73	1.77	5 (11%)	52,89,113	1.62	7 (13%)
21	LMG	J	102	-	55,55,55	0.49	0	63,63,63	0.61	0
15	CLA	B	815	2	65,73,73	1.50	5 (7%)	76,113,113	1.38	8 (10%)
18	BCR	L	209	-	41,41,41	0.30	0	56,56,56	0.66	0
15	CLA	B	824	2	65,73,73	1.47	6 (9%)	76,113,113	1.40	7 (9%)
19	LHG	l	102	-	48,48,48	0.51	0	51,54,54	0.48	0
15	CLA	L	202	10	65,73,73	1.46	6 (9%)	76,113,113	1.40	7 (9%)
15	CLA	A	819	1	65,73,73	1.50	7 (10%)	76,113,113	1.34	8 (10%)
15	CLA	i	103	24	50,58,73	1.71	5 (10%)	58,95,113	1.52	9 (15%)
15	CLA	a	819	1	65,73,73	1.50	7 (10%)	76,113,113	1.34	8 (10%)
15	CLA	a	812	1,15	65,73,73	1.49	5 (7%)	76,113,113	1.34	8 (10%)
14	F6C	a	824	24	55,60,74	2.01	13 (23%)	53,97,114	2.48	15 (28%)
15	CLA	A	814	1	65,73,73	1.46	6 (9%)	76,113,113	1.39	7 (9%)
15	CLA	O	813	2	56,64,73	1.59	7 (12%)	65,102,113	1.49	7 (10%)
15	CLA	B	836	2	65,73,73	1.46	6 (9%)	76,113,113	1.41	9 (11%)
15	CLA	A	805	1,15	60,68,73	1.54	5 (8%)	70,107,113	1.42	7 (10%)
15	CLA	N	835	1	65,73,73	1.49	5 (7%)	76,113,113	1.34	9 (11%)
18	BCR	b	843	-	41,41,41	0.31	0	56,56,56	0.60	0
15	CLA	B	820	24	53,61,73	1.62	6 (11%)	61,98,113	1.56	7 (11%)
15	CLA	N	830	1	65,73,73	1.47	6 (9%)	76,113,113	1.38	6 (7%)
15	CLA	a	814	1	65,73,73	1.46	6 (9%)	76,113,113	1.39	7 (9%)
14	F6C	B	838	24	69,74,74	1.76	13 (18%)	70,114,114	2.28	16 (22%)
15	CLA	b	841	2	65,73,73	1.48	5 (7%)	76,113,113	1.36	8 (10%)
15	CLA	A	827	24	55,63,73	1.59	5 (9%)	64,101,113	1.53	10 (15%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	F6C	b	833	2	69,74,74	1.78	13 (18%)	70,114,114	2.23	17 (24%)
21	LMG	g	103	-	37,37,55	0.56	0	45,45,63	0.66	0
15	CLA	a	811	1	57,65,73	1.56	6 (10%)	66,103,113	1.46	6 (9%)
18	BCR	V	101	-	25,25,41	0.51	1 (4%)	33,33,56	0.52	0
15	CLA	b	812	2	45,53,73	1.79	5 (11%)	52,89,113	1.57	7 (13%)
13	CL0	N	801	1	65,73,73	1.45	6 (9%)	76,113,113	1.38	7 (9%)
15	CLA	N	825	1	65,73,73	1.48	6 (9%)	76,113,113	1.34	8 (10%)
15	CLA	a	830	1	65,73,73	1.46	6 (9%)	76,113,113	1.40	7 (9%)
15	CLA	b	836	24	45,53,73	1.81	5 (11%)	52,89,113	1.54	6 (11%)
15	CLA	B	809	2	65,73,73	1.48	5 (7%)	76,113,113	1.35	8 (10%)
15	CLA	O	838	2	65,73,73	1.46	6 (9%)	76,113,113	1.41	9 (11%)
20	LMT	N	854	-	36,36,36	0.56	0	47,47,47	0.62	0
15	CLA	j	202	10	65,73,73	1.45	6 (9%)	76,113,113	1.39	6 (7%)
17	SF4	c	101	3	0,12,12	-	-	-	-	-
15	CLA	B	814	2	57,65,73	1.56	6 (10%)	66,103,113	1.49	7 (10%)
15	CLA	N	806	1	65,73,73	1.46	5 (7%)	76,113,113	1.42	8 (10%)
15	CLA	N	803	-	65,73,73	1.45	7 (10%)	76,113,113	1.42	8 (10%)
15	CLA	O	820	2	55,63,73	1.62	6 (10%)	64,101,113	1.43	7 (10%)
15	CLA	A	828	1	65,73,73	1.47	6 (9%)	76,113,113	1.37	7 (9%)
15	CLA	N	832	1	50,58,73	1.68	6 (12%)	58,95,113	1.53	8 (13%)
15	CLA	A	812	1,15	65,73,73	1.49	6 (9%)	76,113,113	1.34	8 (10%)
15	CLA	O	837	2	65,73,73	1.46	6 (9%)	76,113,113	1.41	8 (10%)
14	F6C	A	802	24	69,74,74	1.78	13 (18%)	70,114,114	2.17	16 (22%)
18	BCR	J	101	-	41,41,41	0.31	0	56,56,56	0.54	0
14	F6C	L	201	2	69,74,74	1.78	12 (17%)	70,114,114	2.17	16 (22%)
15	CLA	N	831	1	65,73,73	1.47	6 (9%)	76,113,113	1.42	7 (9%)
15	CLA	A	841	1	65,73,73	1.48	6 (9%)	76,113,113	1.37	8 (10%)
22	LFA	f	204	-	15,15,19	0.24	0	14,14,18	0.19	0
15	CLA	N	834	1	65,73,73	1.49	6 (9%)	76,113,113	1.33	8 (10%)
15	CLA	O	816	2	57,65,73	1.56	5 (8%)	66,103,113	1.49	8 (12%)
21	LMG	U	102	-	55,55,55	0.49	0	63,63,63	0.61	0
16	PQN	A	843	-	34,34,34	0.35	0	42,45,45	0.56	0
18	BCR	a	857	-	41,41,41	0.41	0	56,56,56	1.28	8 (14%)
19	LHG	Y	101	-	48,48,48	0.51	0	51,54,54	0.49	0
22	LFA	L	208	-	14,14,19	0.24	0	13,13,18	0.23	0
15	CLA	N	811	1	57,65,73	1.56	7 (12%)	66,103,113	1.47	8 (12%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	CLA	A	839	1	65,73,73	1.48	5 (7%)	76,113,113	1.40	9 (11%)
15	CLA	b	828	2	65,73,73	1.46	6 (9%)	76,113,113	1.36	8 (10%)
15	CLA	N	815	1	55,63,73	1.61	6 (10%)	64,101,113	1.49	8 (12%)
16	PQN	B	840	-	34,34,34	0.35	0	42,45,45	0.59	1 (2%)
21	LMG	N	855	-	44,44,55	0.53	0	52,52,63	0.65	0
15	CLA	j	203	10	60,68,73	1.54	5 (8%)	70,107,113	1.43	10 (14%)
18	BCR	O	847	-	41,41,41	0.32	0	56,56,56	0.84	3 (5%)
20	LMT	a	854	-	36,36,36	0.56	0	47,47,47	0.63	0
18	BCR	A	858	-	41,41,41	0.42	0	56,56,56	1.30	8 (14%)
18	BCR	W	1508	-	41,41,41	0.30	0	56,56,56	0.66	0
15	CLA	a	806	1	65,73,73	1.46	6 (9%)	76,113,113	1.40	7 (9%)
15	CLA	A	856	24	65,73,73	1.48	6 (9%)	76,113,113	1.38	7 (9%)
15	CLA	b	815	2	45,53,73	1.78	5 (11%)	52,89,113	1.65	8 (15%)
18	BCR	N	845	-	41,41,41	0.35	0	56,56,56	0.92	0
15	CLA	A	836	1	54,62,73	1.61	6 (11%)	62,99,113	1.51	8 (12%)
18	BCR	B	842	-	41,41,41	0.31	0	56,56,56	0.64	0
15	CLA	O	836	24	45,53,73	1.80	5 (11%)	52,89,113	1.55	6 (11%)
14	F6C	A	857	24	69,74,74	1.75	13 (18%)	70,114,114	2.29	16 (22%)
15	CLA	N	816	1	45,53,73	1.80	5 (11%)	52,89,113	1.57	7 (13%)
17	SF4	P	101	3	0,12,12	-	-	-		
17	SF4	C	101	3	0,12,12	-	-	-		
15	CLA	N	839	1	65,73,73	1.48	5 (7%)	76,113,113	1.39	9 (11%)
15	CLA	B	825	2	62,70,73	1.51	6 (9%)	72,109,113	1.38	7 (9%)
18	BCR	b	845	-	41,41,41	0.30	0	56,56,56	0.47	0
22	LFA	O	851	-	15,15,19	0.23	0	14,14,18	0.19	0
15	CLA	b	804	2	65,73,73	1.48	6 (9%)	76,113,113	1.37	8 (10%)
21	LMG	j	206	-	50,50,55	0.50	0	58,58,63	0.60	0
15	CLA	A	817	24	45,53,73	1.81	5 (11%)	52,89,113	1.59	6 (11%)
13	CL0	a	801	1	65,73,73	1.45	6 (9%)	76,113,113	1.38	7 (9%)
15	CLA	S	201	24	65,73,73	1.49	6 (9%)	76,113,113	1.33	8 (10%)
15	CLA	b	830	2	65,73,73	1.47	6 (9%)	76,113,113	1.35	6 (7%)
14	F6C	O	840	24	69,74,74	1.76	13 (18%)	70,114,114	2.27	16 (22%)
18	BCR	T	101	-	41,41,41	0.33	0	56,56,56	0.73	0
19	LHG	M	102	-	48,48,48	0.51	0	51,54,54	0.50	0
15	CLA	N	840	1	50,58,73	1.68	5 (10%)	58,95,113	1.55	8 (13%)
15	CLA	B	813	2	45,53,73	1.75	6 (13%)	52,89,113	1.65	7 (13%)
14	F6C	b	810	2	69,74,74	1.79	11 (15%)	70,114,114	2.16	15 (21%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
21	LMG	B	847	-	55,55,55	0.50	0	63,63,63	0.60	0
15	CLA	a	807	1	65,73,73	1.48	6 (9%)	76,113,113	1.38	7 (9%)
14	F6C	O	810	2	69,74,74	1.78	11 (15%)	70,114,114	2.17	14 (20%)
15	CLA	B	822	24	65,73,73	1.47	6 (9%)	76,113,113	1.44	9 (11%)
15	CLA	A	821	1	60,68,73	1.54	6 (10%)	70,107,113	1.41	7 (10%)
17	SF4	N	844	1,2	0,12,12	-	-	-	-	-
14	F6C	b	840	24	69,74,74	1.76	13 (18%)	70,114,114	2.28	16 (22%)
15	CLA	O	825	24	65,73,73	1.47	5 (7%)	76,113,113	1.43	8 (10%)
18	BCR	U	101	-	41,41,41	0.32	0	56,56,56	0.54	0
15	CLA	A	831	1	65,73,73	1.47	6 (9%)	76,113,113	1.38	7 (9%)
15	CLA	N	809	1	60,68,73	1.53	5 (8%)	70,107,113	1.40	8 (11%)
15	CLA	X	103	12	55,63,73	1.61	6 (10%)	64,101,113	1.46	7 (10%)
15	CLA	B	830	2	65,73,73	1.48	5 (7%)	76,113,113	1.40	8 (10%)
15	CLA	O	817	2	65,73,73	1.50	5 (7%)	76,113,113	1.37	8 (10%)
15	CLA	N	807	1	65,73,73	1.48	6 (9%)	76,113,113	1.37	7 (9%)
15	CLA	a	835	1	65,73,73	1.48	5 (7%)	76,113,113	1.35	9 (11%)
18	BCR	a	850	-	41,41,41	0.33	0	56,56,56	0.87	0
15	CLA	O	802	24	65,73,73	1.47	5 (7%)	76,113,113	1.37	7 (9%)
15	CLA	O	822	24	53,61,73	1.62	5 (9%)	61,98,113	1.57	7 (11%)
18	BCR	B	844	-	41,41,41	0.31	0	56,56,56	0.61	0
18	BCR	O	849	-	41,41,41	0.30	0	56,56,56	0.60	0
19	LHG	A	851	-	41,41,48	0.55	0	44,47,54	0.51	0
15	CLA	A	818	1	65,73,73	1.45	7 (10%)	76,113,113	1.45	9 (11%)
21	LMG	T	103	-	37,37,55	0.55	0	45,45,63	0.66	0
15	CLA	B	807	2	65,73,73	1.45	7 (10%)	76,113,113	1.44	9 (11%)
15	CLA	O	808	2	65,73,73	1.45	6 (9%)	76,113,113	1.45	9 (11%)
15	CLA	O	831	2	65,73,73	1.47	6 (9%)	76,113,113	1.39	9 (11%)
15	CLA	a	818	1	65,73,73	1.46	7 (10%)	76,113,113	1.42	9 (11%)
15	CLA	a	834	1	65,73,73	1.49	6 (9%)	76,113,113	1.33	7 (9%)
19	LHG	X	102	-	48,48,48	0.51	0	51,54,54	0.48	0
15	CLA	B	802	-	65,73,73	1.46	7 (10%)	76,113,113	1.42	7 (9%)
15	CLA	b	832	2	65,73,73	1.47	5 (7%)	76,113,113	1.40	8 (10%)
18	BCR	g	102	-	41,41,41	0.29	0	56,56,56	0.49	0
15	CLA	B	835	2	65,73,73	1.46	6 (9%)	76,113,113	1.41	8 (10%)
15	CLA	A	822	24	65,73,73	1.49	6 (9%)	76,113,113	1.36	7 (9%)
15	CLA	b	838	2	65,73,73	1.45	6 (9%)	76,113,113	1.41	9 (11%)
15	CLA	b	837	2	65,73,73	1.46	6 (9%)	76,113,113	1.41	7 (9%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	LHG	L	207	-	48,48,48	0.51	0	51,54,54	0.48	0
15	CLA	A	810	1	57,65,73	1.56	6 (10%)	66,103,113	1.52	8 (12%)
15	CLA	N	818	1	65,73,73	1.46	7 (10%)	76,113,113	1.44	9 (11%)
15	CLA	A	833	1	55,63,73	1.59	6 (10%)	64,101,113	1.52	7 (10%)
15	CLA	a	803	-	65,73,73	1.45	7 (10%)	76,113,113	1.41	7 (9%)
20	LMT	a	853	-	29,29,36	0.57	0	40,40,47	1.42	5 (12%)
18	BCR	k	102	-	41,41,41	0.32	0	56,56,56	0.68	1 (1%)
18	BCR	A	848	-	41,41,41	0.31	0	56,56,56	0.52	0
15	CLA	b	825	24	65,73,73	1.47	5 (7%)	76,113,113	1.44	9 (11%)
18	BCR	S	202	-	41,41,41	0.30	0	56,56,56	0.51	0
15	CLA	b	824	24	65,73,73	1.47	6 (9%)	76,113,113	1.43	9 (11%)
13	CL0	A	801	1	65,73,73	1.45	6 (9%)	76,113,113	1.38	7 (9%)
15	CLA	a	842	1	65,73,73	1.50	5 (7%)	76,113,113	1.34	8 (10%)
18	BCR	I	101	-	41,41,41	0.34	0	56,56,56	0.74	0
15	CLA	b	806	2	65,73,73	1.45	6 (9%)	76,113,113	1.43	6 (7%)
15	CLA	A	838	1	55,63,73	1.58	6 (10%)	64,101,113	1.47	7 (10%)
15	CLA	A	807	1	65,73,73	1.47	6 (9%)	76,113,113	1.38	6 (7%)
19	LHG	k	101	-	48,48,48	0.50	0	51,54,54	0.50	0
15	CLA	B	811	2	56,64,73	1.59	7 (12%)	65,102,113	1.49	7 (10%)
15	CLA	B	829	2	65,73,73	1.47	6 (9%)	76,113,113	1.38	9 (11%)
15	CLA	N	833	1	55,63,73	1.59	6 (10%)	64,101,113	1.52	7 (10%)
17	SF4	a	844	1,2	0,12,12	-	-	-	-	-
15	CLA	O	841	2	65,73,73	1.49	5 (7%)	76,113,113	1.36	8 (10%)
15	CLA	A	820	1	65,73,73	1.47	5 (7%)	76,113,113	1.49	10 (13%)
15	CLA	B	839	2	65,73,73	1.48	6 (9%)	76,113,113	1.37	8 (10%)
14	F6C	O	833	2	69,74,74	1.79	13 (18%)	70,114,114	2.22	16 (22%)
15	CLA	B	826	2	65,73,73	1.46	6 (9%)	76,113,113	1.36	8 (10%)
14	F6C	N	856	24	69,74,74	1.75	13 (18%)	70,114,114	2.27	16 (22%)
19	LHG	l	101	-	43,43,48	0.54	0	46,49,54	0.50	0
15	CLA	a	839	1	65,73,73	1.48	5 (7%)	76,113,113	1.39	8 (10%)
15	CLA	O	821	2	45,53,73	1.77	5 (11%)	52,89,113	1.62	7 (13%)
15	CLA	B	823	24	65,73,73	1.47	5 (7%)	76,113,113	1.44	8 (10%)
20	LMT	A	852	-	32,32,36	0.57	0	43,43,47	0.67	0
21	LMG	a	855	-	44,44,55	0.52	0	52,52,63	0.62	0
15	CLA	O	807	2	65,73,73	1.47	6 (9%)	76,113,113	1.37	8 (10%)
14	F6C	L	204	24	69,74,74	1.78	14 (20%)	70,114,114	2.25	18 (25%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	CLA	a	823	1	56,64,73	1.59	5 (8%)	65,102,113	1.48	6 (9%)
15	CLA	O	804	2	65,73,73	1.48	6 (9%)	76,113,113	1.37	8 (10%)
15	CLA	N	820	1	65,73,73	1.46	5 (7%)	76,113,113	1.51	10 (13%)
18	BCR	i	101	-	25,25,41	0.51	1 (4%)	33,33,56	0.51	0
15	CLA	a	829	1	60,68,73	1.53	6 (10%)	70,107,113	1.42	7 (10%)
14	F6C	a	856	24	69,74,74	1.75	13 (18%)	70,114,114	2.27	16 (22%)
15	CLA	b	809	2	65,73,73	1.48	6 (9%)	76,113,113	1.36	8 (10%)
21	LMG	h	102	-	55,55,55	0.49	0	63,63,63	0.62	0
15	CLA	b	826	2	65,73,73	1.47	6 (9%)	76,113,113	1.41	7 (9%)
15	CLA	b	807	2	65,73,73	1.48	6 (9%)	76,113,113	1.37	9 (11%)
15	CLA	B	816	2	60,68,73	1.55	5 (8%)	70,107,113	1.39	7 (10%)
15	CLA	b	814	2	65,73,73	1.48	6 (9%)	76,113,113	1.36	8 (10%)
18	BCR	f	203	-	41,41,41	0.31	0	56,56,56	0.48	0
15	CLA	b	820	2	55,63,73	1.62	6 (10%)	64,101,113	1.43	7 (10%)
15	CLA	a	816	1	45,53,73	1.80	5 (11%)	52,89,113	1.57	7 (13%)
15	CLA	N	829	1	60,68,73	1.53	6 (10%)	70,107,113	1.42	8 (11%)
15	CLA	B	803	2	65,73,73	1.48	6 (9%)	76,113,113	1.37	8 (10%)
14	F6C	N	802	24	69,74,74	1.77	13 (18%)	70,114,114	2.17	15 (21%)
15	CLA	Z	103	12	55,63,73	1.61	6 (10%)	64,101,113	1.46	7 (10%)
18	BCR	h	101	-	41,41,41	0.31	0	56,56,56	0.54	0
20	LMT	N	853	-	29,29,36	0.57	0	40,40,47	1.41	5 (12%)
15	CLA	B	832	2	55,63,73	1.60	6 (10%)	64,101,113	1.47	7 (10%)
15	CLA	b	811	2	65,73,73	1.47	5 (7%)	76,113,113	1.37	8 (10%)
15	CLA	O	823	2	55,63,73	1.60	7 (12%)	64,101,113	1.51	9 (14%)
18	BCR	a	848	-	41,41,41	0.32	0	56,56,56	0.51	0
15	CLA	A	837	1	51,59,73	1.67	5 (9%)	59,96,113	1.51	8 (13%)
15	CLA	L	203	10	60,68,73	1.54	5 (8%)	70,107,113	1.43	10 (14%)
15	CLA	B	837	2	65,73,73	1.47	6 (9%)	76,113,113	1.42	8 (10%)
15	CLA	b	819	24	65,73,73	1.51	6 (9%)	76,113,113	1.35	8 (10%)
15	CLA	A	840	1	50,58,73	1.68	5 (10%)	58,95,113	1.56	8 (13%)
15	CLA	O	812	2	45,53,73	1.78	5 (11%)	52,89,113	1.57	7 (13%)
18	BCR	N	850	-	41,41,41	0.32	0	56,56,56	0.86	0
15	CLA	a	813	1	54,62,73	1.61	5 (9%)	62,99,113	1.52	9 (14%)
18	BCR	a	847	-	41,41,41	0.31	0	56,56,56	0.61	1 (1%)
14	F6C	a	802	24	69,74,74	1.77	13 (18%)	70,114,114	2.17	14 (20%)
15	CLA	N	836	1	54,62,73	1.61	6 (11%)	62,99,113	1.51	8 (12%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
21	LMG	O	850	-	55,55,55	0.49	0	63,63,63	0.60	0
15	CLA	O	828	2	65,73,73	1.45	6 (9%)	76,113,113	1.38	8 (10%)
15	CLA	B	819	2	45,53,73	1.77	5 (11%)	52,89,113	1.61	7 (13%)
18	BCR	B	846	-	41,41,41	0.30	0	56,56,56	0.61	0
15	CLA	a	841	1	65,73,73	1.48	7 (10%)	76,113,113	1.37	8 (10%)
18	BCR	N	847	-	41,41,41	0.31	0	56,56,56	0.60	1 (1%)
15	CLA	f	201	24	65,73,73	1.49	6 (9%)	76,113,113	1.33	8 (10%)
18	BCR	K	101	-	25,25,41	0.51	1 (4%)	33,33,56	0.51	0
15	CLA	B	818	2	55,63,73	1.62	6 (10%)	64,101,113	1.43	7 (10%)
15	CLA	A	842	1	65,73,73	1.50	6 (9%)	76,113,113	1.33	8 (10%)
15	CLA	B	834	24	45,53,73	1.80	5 (11%)	52,89,113	1.55	6 (11%)
15	CLA	F	201	24	65,73,73	1.49	6 (9%)	76,113,113	1.33	8 (10%)
16	PQN	N	843	-	34,34,34	0.34	0	42,45,45	0.52	0
21	LMG	W	1505	-	50,50,55	0.50	0	58,58,63	0.60	0
15	CLA	O	824	24	65,73,73	1.48	6 (9%)	76,113,113	1.43	9 (11%)
21	LMG	L	206	-	50,50,55	0.50	0	58,58,63	0.60	0
18	BCR	B	843	-	41,41,41	0.30	0	56,56,56	0.48	0
18	BCR	b	846	-	41,41,41	0.31	0	56,56,56	0.58	0
19	LHG	N	851	-	41,41,48	0.55	0	44,47,54	0.50	0
18	BCR	O	846	-	41,41,41	0.31	0	56,56,56	0.60	0
15	CLA	a	805	1,15	60,68,73	1.54	5 (8%)	70,107,113	1.42	8 (11%)
15	CLA	b	818	2	60,68,73	1.55	5 (8%)	70,107,113	1.38	7 (10%)
14	F6C	A	824	24	55,60,74	2.01	14 (25%)	53,97,114	2.48	15 (28%)
15	CLA	b	801	2	65,73,73	1.47	7 (10%)	76,113,113	1.32	8 (10%)
18	BCR	B	841	-	41,41,41	0.31	0	56,56,56	0.60	0
20	LMT	a	852	-	32,32,36	0.57	0	43,43,47	0.68	0
15	CLA	W	1501	10	65,73,73	1.47	6 (9%)	76,113,113	1.38	6 (7%)
14	F6C	A	826	24	69,74,74	1.79	12 (17%)	70,114,114	2.28	18 (25%)
15	CLA	a	836	1	54,62,73	1.61	6 (11%)	62,99,113	1.51	8 (12%)
19	LHG	W	1506	-	48,48,48	0.51	0	51,54,54	0.47	0
18	BCR	a	849	-	41,41,41	0.32	0	56,56,56	0.59	0
15	CLA	N	812	1,15	65,73,73	1.49	5 (7%)	76,113,113	1.34	8 (10%)
15	CLA	O	819	24	65,73,73	1.51	5 (7%)	76,113,113	1.34	8 (10%)
14	F6C	W	1503	24	69,74,74	1.77	12 (17%)	70,114,114	2.26	17 (24%)
15	CLA	K	103	24	50,58,73	1.71	5 (10%)	58,95,113	1.55	9 (15%)
18	BCR	N	846	-	41,41,41	0.33	0	56,56,56	0.68	1 (1%)
15	CLA	a	808	1	45,53,73	1.76	5 (11%)	52,89,113	1.64	8 (15%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	LFA	j	208	-	14,14,19	0.24	0	13,13,18	0.23	0
15	CLA	a	831	1	65,73,73	1.48	5 (7%)	76,113,113	1.38	7 (9%)
15	CLA	a	833	1	55,63,73	1.58	6 (10%)	64,101,113	1.51	7 (10%)
15	CLA	A	809	1	60,68,73	1.53	5 (8%)	70,107,113	1.41	8 (11%)
18	BCR	O	848	-	41,41,41	0.32	0	56,56,56	0.99	4 (7%)
15	CLA	a	821	1	60,68,73	1.54	6 (10%)	70,107,113	1.41	7 (10%)
15	CLA	A	804	1	65,73,73	1.50	6 (9%)	76,113,113	1.37	7 (9%)
18	BCR	g	101	-	41,41,41	0.33	0	56,56,56	0.70	0
18	BCR	A	846	-	41,41,41	0.33	0	56,56,56	0.66	1 (1%)
15	CLA	O	803	-	65,73,73	1.46	7 (10%)	76,113,113	1.40	7 (9%)
15	CLA	l	103	12	55,63,73	1.60	6 (10%)	64,101,113	1.46	7 (10%)
15	CLA	N	810	1	57,65,73	1.56	6 (10%)	66,103,113	1.52	7 (10%)
17	SF4	c	102	3	0,12,12	-	-	-	-	-
15	CLA	O	832	2	65,73,73	1.48	5 (7%)	76,113,113	1.41	8 (10%)
16	PQN	a	843	-	34,34,34	0.34	0	42,45,45	0.56	1 (2%)
18	BCR	j	205	-	41,41,41	0.33	0	56,56,56	0.67	0
19	LHG	a	851	-	41,41,48	0.55	0	44,47,54	0.52	0
18	BCR	W	1504	-	41,41,41	0.33	0	56,56,56	0.57	0
15	CLA	O	827	2	62,70,73	1.52	6 (9%)	72,109,113	1.39	7 (9%)
15	CLA	b	835	24	45,53,73	1.77	6 (13%)	52,89,113	1.62	6 (11%)
15	CLA	B	812	2	65,73,73	1.48	6 (9%)	76,113,113	1.37	8 (10%)
18	BCR	O	845	-	41,41,41	0.30	0	56,56,56	0.47	0
15	CLA	N	804	1	65,73,73	1.50	6 (9%)	76,113,113	1.37	7 (9%)
15	CLA	O	806	2	65,73,73	1.46	6 (9%)	76,113,113	1.44	7 (9%)
18	BCR	j	201	-	41,41,41	0.30	0	56,56,56	0.67	0
19	LHG	X	101	-	43,43,48	0.54	0	46,49,54	0.51	0
15	CLA	N	822	24	65,73,73	1.50	6 (9%)	76,113,113	1.34	7 (9%)
15	CLA	b	834	2	55,63,73	1.60	6 (10%)	64,101,113	1.47	7 (10%)
18	BCR	N	849	-	41,41,41	0.32	0	56,56,56	0.59	0
18	BCR	O	843	-	41,41,41	0.31	0	56,56,56	0.60	0
15	CLA	A	825	1	65,73,73	1.49	6 (9%)	76,113,113	1.34	8 (10%)
15	CLA	N	837	1	51,59,73	1.67	5 (9%)	59,96,113	1.52	9 (15%)
19	LHG	Z	102	-	48,48,48	0.51	0	51,54,54	0.48	0
15	CLA	B	806	2	65,73,73	1.46	6 (9%)	76,113,113	1.39	9 (11%)
18	BCR	Y	102	-	41,41,41	0.32	0	56,56,56	0.65	1 (1%)
15	CLA	N	827	24	55,63,73	1.60	5 (9%)	64,101,113	1.51	9 (14%)
15	CLA	N	808	1	45,53,73	1.76	6 (13%)	52,89,113	1.66	8 (15%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	CLA	N	805	1,15	60,68,73	1.54	5 (8%)	70,107,113	1.42	7 (10%)
15	CLA	O	829	2	65,73,73	1.47	5 (7%)	76,113,113	1.43	8 (10%)
19	LHG	j	207	-	48,48,48	0.51	0	51,54,54	0.48	0
15	CLA	b	803	-	65,73,73	1.46	7 (10%)	76,113,113	1.43	7 (9%)
15	CLA	A	803	-	65,73,73	1.45	7 (10%)	76,113,113	1.41	8 (10%)
14	F6C	j	204	24	69,74,74	1.77	13 (18%)	70,114,114	2.27	18 (25%)
15	CLA	A	830	1	65,73,73	1.46	6 (9%)	76,113,113	1.39	6 (7%)
15	CLA	A	815	1	55,63,73	1.61	6 (10%)	64,101,113	1.49	8 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	a	822	24	1/1/15/20	16/37/115/115	-
18	BCR	O	844	-	-	5/29/63/63	0/2/2/2
20	LMT	N	852	-	-	3/17/57/61	0/2/2/2
18	BCR	F	202	-	-	7/29/63/63	0/2/2/2
15	CLA	O	826	2	1/1/15/20	4/37/115/115	-
15	CLA	O	814	2	1/1/15/20	15/37/115/115	-
22	LFA	B	848	-	-	6/13/13/17	-
15	CLA	N	828	1	1/1/15/20	5/37/115/115	-
15	CLA	b	817	2	1/1/15/20	9/37/115/115	-
15	CLA	a	825	1	1/1/15/20	9/37/115/115	-
15	CLA	a	817	24	1/1/11/20	5/13/91/115	-
15	CLA	b	816	2	1/1/13/20	7/28/106/115	-
15	CLA	A	806	1	1/1/15/20	19/37/115/115	-
15	CLA	O	835	24	1/1/11/20	2/13/91/115	-
15	CLA	a	809	1	1/1/14/20	10/31/109/115	-
15	CLA	b	839	2	1/1/15/20	11/37/115/115	-
15	CLA	b	805	2	1/1/15/20	13/37/115/115	-
20	LMT	A	854	-	-	5/21/61/61	0/2/2/2
15	CLA	N	841	1	1/1/15/20	17/37/115/115	-
21	LMG	b	849	-	-	7/50/70/70	0/1/1/1
15	CLA	K	102	9	1/1/11/20	6/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BCR	M	101	-	-	7/29/63/63	0/2/2/2
15	CLA	O	815	2	1/1/11/20	7/13/91/115	-
15	CLA	W	1502	10	1/1/14/20	12/31/109/115	-
15	CLA	b	823	2	1/1/13/20	8/25/103/115	-
15	CLA	O	830	2	1/1/15/20	16/37/115/115	-
15	CLA	a	840	1	1/1/12/20	2/19/97/115	-
15	CLA	b	827	2	1/1/14/20	17/34/112/115	-
18	BCR	A	849	-	-	3/29/63/63	0/2/2/2
21	LMG	I	103	-	-	11/32/52/70	0/1/1/1
15	CLA	A	832	1	1/1/12/20	5/19/97/115	-
15	CLA	N	821	1	1/1/14/20	8/31/109/115	-
18	BCR	T	102	-	-	4/29/63/63	0/2/2/2
15	CLA	A	835	1	1/1/15/20	10/37/115/115	-
15	CLA	V	103	24	1/1/12/20	2/19/97/115	-
18	BCR	I	102	-	-	4/29/63/63	0/2/2/2
18	BCR	A	850	-	-	14/29/63/63	0/2/2/2
15	CLA	a	810	1	1/1/13/20	9/28/106/115	-
15	CLA	b	808	2	1/1/15/20	11/37/115/115	-
18	BCR	b	848	-	-	3/29/63/63	0/2/2/2
15	CLA	N	823	1	1/1/13/20	6/27/105/115	-
18	BCR	a	845	-	-	3/29/63/63	0/2/2/2
15	CLA	O	811	2	1/1/15/20	11/37/115/115	-
18	BCR	A	847	-	-	6/29/63/63	0/2/2/2
15	CLA	a	804	1	1/1/15/20	6/37/115/115	-
15	CLA	B	810	2	1/1/11/20	4/13/91/115	-
15	CLA	b	813	2	-	11/27/105/115	-
18	BCR	b	847	-	-	1/29/63/63	0/2/2/2
14	F6C	N	824	24	-	11/25/81/97	-
15	CLA	N	817	24	1/1/11/20	5/13/91/115	-
15	CLA	b	831	2	1/1/15/20	11/37/115/115	-
15	CLA	O	809	2	1/1/15/20	15/37/115/115	-
15	CLA	O	818	2	1/1/14/20	13/31/109/115	-
15	CLA	O	834	2	1/1/13/20	8/25/103/115	-
15	CLA	N	814	1	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	a	827	24	1/1/13/20	2/25/103/115	-
16	PQN	O	842	-	-	0/23/43/43	0/2/2/2
21	LMG	A	855	-	-	9/39/59/70	0/1/1/1
15	CLA	a	820	1	1/1/15/20	20/37/115/115	-
15	CLA	A	823	1	1/1/13/20	6/27/105/115	-
18	BCR	N	848	-	-	8/29/63/63	0/2/2/2
18	BCR	B	845	-	-	2/29/63/63	0/2/2/2
15	CLA	B	821	2	1/1/13/20	12/25/103/115	-
15	CLA	N	838	1	1/1/13/20	12/25/103/115	-
15	CLA	B	804	2	1/1/15/20	15/37/115/115	-
18	BCR	F	203	-	-	2/29/63/63	0/2/2/2
17	SF4	A	844	1,2	-	-	0/6/5/5
15	CLA	i	102	9	1/1/11/20	6/13/91/115	-
16	PQN	b	842	-	-	0/23/43/43	0/2/2/2
15	CLA	N	813	1	1/1/12/20	9/24/102/115	-
15	CLA	B	808	2	1/1/15/20	13/37/115/115	-
15	CLA	B	805	2	1/1/15/20	16/37/115/115	-
15	CLA	O	805	2	1/1/15/20	11/37/115/115	-
22	LFA	W	1507	-	-	0/12/12/17	-
15	CLA	A	808	1	1/1/11/20	1/13/91/115	-
15	CLA	B	827	2	1/1/15/20	12/37/115/115	-
18	BCR	N	857	-	-	9/29/63/63	0/2/2/2
15	CLA	A	811	1	1/1/13/20	12/28/106/115	-
15	CLA	A	813	1	1/1/12/20	8/24/102/115	-
14	F6C	N	826	24	-	16/41/97/97	-
15	CLA	a	832	1	1/1/12/20	5/19/97/115	-
19	LHG	Z	101	-	-	22/48/48/53	-
18	BCR	L	205	-	-	4/29/63/63	0/2/2/2
18	BCR	f	202	-	-	7/29/63/63	0/2/2/2
15	CLA	a	837	1	1/1/12/20	9/21/99/115	-
15	CLA	B	801	2	1/1/15/20	12/37/115/115	-
18	BCR	A	845	-	-	3/29/63/63	0/2/2/2
15	CLA	O	801	2	1/1/15/20	12/37/115/115	-
18	BCR	b	844	-	-	5/29/63/63	0/2/2/2
15	CLA	O	839	2	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	N	842	1	1/1/15/20	10/37/115/115	-
15	CLA	a	815	1	1/1/13/20	5/25/103/115	-
15	CLA	A	816	1	1/1/11/20	8/13/91/115	-
15	CLA	A	834	1	1/1/15/20	5/37/115/115	-
15	CLA	B	817	24	1/1/15/20	8/37/115/115	-
15	CLA	B	828	2	1/1/15/20	19/37/115/115	-
15	CLA	b	802	24	1/1/15/20	14/37/115/115	-
15	CLA	b	822	24	1/1/12/20	9/23/101/115	-
15	CLA	B	833	24	1/1/11/20	2/13/91/115	-
20	LMT	A	853	-	-	10/14/54/61	0/2/2/2
15	CLA	a	828	1	1/1/15/20	9/37/115/115	-
18	BCR	a	846	-	-	8/29/63/63	0/2/2/2
14	F6C	a	826	24	-	14/41/97/97	-
17	SF4	P	102	3	-	-	0/6/5/5
17	SF4	C	102	3	-	-	0/6/5/5
15	CLA	V	102	9	1/1/11/20	6/13/91/115	-
15	CLA	b	829	2	1/1/15/20	11/37/115/115	-
15	CLA	N	819	1	1/1/15/20	10/37/115/115	-
15	CLA	a	838	1	1/1/13/20	12/25/103/115	-
15	CLA	A	829	1	1/1/14/20	15/31/109/115	-
15	CLA	b	821	2	1/1/11/20	7/13/91/115	-
14	F6C	B	831	2	-	7/41/97/97	-
21	LMG	J	102	-	-	19/50/70/70	0/1/1/1
15	CLA	B	815	2	1/1/15/20	11/37/115/115	-
18	BCR	L	209	-	-	2/29/63/63	0/2/2/2
15	CLA	B	824	2	1/1/15/20	5/37/115/115	-
19	LHG	l	102	-	-	21/53/53/53	-
15	CLA	L	202	10	1/1/15/20	7/37/115/115	-
15	CLA	A	819	1	1/1/15/20	9/37/115/115	-
15	CLA	i	103	24	1/1/12/20	2/19/97/115	-
15	CLA	a	819	1	1/1/15/20	14/37/115/115	-
15	CLA	a	812	1,15	1/1/15/20	19/37/115/115	-
14	F6C	a	824	24	-	9/25/81/97	-
15	CLA	A	814	1	1/1/15/20	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	O	813	2	-	10/27/105/115	-
15	CLA	B	836	2	1/1/15/20	12/37/115/115	-
15	CLA	A	805	1,15	1/1/14/20	10/31/109/115	-
15	CLA	N	835	1	1/1/15/20	12/37/115/115	-
18	BCR	b	843	-	-	3/29/63/63	0/2/2/2
15	CLA	B	820	24	1/1/12/20	10/23/101/115	-
15	CLA	N	830	1	1/1/15/20	7/37/115/115	-
15	CLA	a	814	1	1/1/15/20	9/37/115/115	-
14	F6C	B	838	24	-	14/41/97/97	-
15	CLA	b	841	2	1/1/15/20	13/37/115/115	-
15	CLA	A	827	24	1/1/13/20	1/25/103/115	-
14	F6C	b	833	2	-	5/41/97/97	-
21	LMG	g	103	-	-	15/32/52/70	0/1/1/1
15	CLA	a	811	1	1/1/13/20	13/28/106/115	-
18	BCR	V	101	-	-	0/18/35/63	0/1/1/2
15	CLA	b	812	2	1/1/11/20	4/13/91/115	-
13	CL0	N	801	1	3/3/20/25	9/37/135/135	-
15	CLA	N	825	1	1/1/15/20	9/37/115/115	-
15	CLA	a	830	1	1/1/15/20	6/37/115/115	-
15	CLA	b	836	24	1/1/11/20	10/13/91/115	-
15	CLA	B	809	2	1/1/15/20	11/37/115/115	-
15	CLA	O	838	2	1/1/15/20	10/37/115/115	-
20	LMT	N	854	-	-	4/21/61/61	0/2/2/2
15	CLA	j	202	10	1/1/15/20	6/37/115/115	-
17	SF4	c	101	3	-	-	0/6/5/5
15	CLA	B	814	2	1/1/13/20	5/28/106/115	-
15	CLA	N	806	1	1/1/15/20	19/37/115/115	-
15	CLA	N	803	-	1/1/15/20	12/37/115/115	-
15	CLA	O	820	2	1/1/13/20	11/25/103/115	-
15	CLA	A	828	1	1/1/15/20	8/37/115/115	-
15	CLA	N	832	1	1/1/12/20	3/19/97/115	-
15	CLA	A	812	1,15	1/1/15/20	20/37/115/115	-
15	CLA	O	837	2	1/1/15/20	10/37/115/115	-
14	F6C	A	802	24	-	9/41/97/97	-
18	BCR	J	101	-	-	7/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	F6C	L	201	2	-	9/41/97/97	-
15	CLA	N	831	1	1/1/15/20	13/37/115/115	-
15	CLA	A	841	1	1/1/15/20	14/37/115/115	-
22	LFA	f	204	-	-	6/13/13/17	-
15	CLA	N	834	1	1/1/15/20	7/37/115/115	-
15	CLA	O	816	2	1/1/13/20	5/28/106/115	-
21	LMG	U	102	-	-	19/50/70/70	0/1/1/1
16	PQN	A	843	-	-	0/23/43/43	0/2/2/2
18	BCR	a	857	-	-	10/29/63/63	0/2/2/2
19	LHG	Y	101	-	-	18/53/53/53	-
22	LFA	L	208	-	-	0/12/12/17	-
15	CLA	N	811	1	1/1/13/20	13/28/106/115	-
15	CLA	A	839	1	1/1/15/20	14/37/115/115	-
15	CLA	b	828	2	1/1/15/20	13/37/115/115	-
15	CLA	N	815	1	1/1/13/20	3/25/103/115	-
16	PQN	B	840	-	-	0/23/43/43	0/2/2/2
21	LMG	N	855	-	-	5/39/59/70	0/1/1/1
15	CLA	j	203	10	1/1/14/20	12/31/109/115	-
18	BCR	O	847	-	-	1/29/63/63	0/2/2/2
20	LMT	a	854	-	-	4/21/61/61	0/2/2/2
18	BCR	A	858	-	-	10/29/63/63	0/2/2/2
18	BCR	W	1508	-	-	2/29/63/63	0/2/2/2
15	CLA	a	806	1	1/1/15/20	18/37/115/115	-
15	CLA	A	856	24	1/1/15/20	15/37/115/115	-
15	CLA	b	815	2	1/1/11/20	6/13/91/115	-
18	BCR	N	845	-	-	3/29/63/63	0/2/2/2
15	CLA	A	836	1	1/1/12/20	8/24/102/115	-
18	BCR	B	842	-	-	5/29/63/63	0/2/2/2
15	CLA	O	836	24	1/1/11/20	10/13/91/115	-
14	F6C	A	857	24	-	19/41/97/97	-
15	CLA	N	816	1	1/1/11/20	9/13/91/115	-
17	SF4	P	101	3	-	-	0/6/5/5
17	SF4	C	101	3	-	-	0/6/5/5
15	CLA	N	839	1	1/1/15/20	18/37/115/115	-
15	CLA	B	825	2	1/1/14/20	16/34/112/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BCR	b	845	-	-	4/29/63/63	0/2/2/2
22	LFA	O	851	-	-	6/13/13/17	-
15	CLA	b	804	2	1/1/15/20	8/37/115/115	-
21	LMG	j	206	-	-	10/45/65/70	0/1/1/1
15	CLA	A	817	24	1/1/11/20	5/13/91/115	-
13	CL0	a	801	1	3/3/20/25	8/37/135/135	-
15	CLA	S	201	24	1/1/15/20	8/37/115/115	-
15	CLA	b	830	2	1/1/15/20	16/37/115/115	-
14	F6C	O	840	24	-	14/41/97/97	-
18	BCR	T	101	-	-	9/29/63/63	0/2/2/2
19	LHG	M	102	-	-	18/53/53/53	-
15	CLA	N	840	1	1/1/12/20	2/19/97/115	-
15	CLA	B	813	2	1/1/11/20	7/13/91/115	-
14	F6C	b	810	2	-	8/41/97/97	-
21	LMG	B	847	-	-	7/50/70/70	0/1/1/1
15	CLA	a	807	1	1/1/15/20	15/37/115/115	-
14	F6C	O	810	2	-	8/41/97/97	-
15	CLA	B	822	24	1/1/15/20	9/37/115/115	-
15	CLA	A	821	1	1/1/14/20	8/31/109/115	-
17	SF4	N	844	1,2	-	-	0/6/5/5
14	F6C	b	840	24	-	14/41/97/97	-
15	CLA	O	825	24	1/1/15/20	14/37/115/115	-
18	BCR	U	101	-	-	7/29/63/63	0/2/2/2
15	CLA	A	831	1	1/1/15/20	12/37/115/115	-
15	CLA	N	809	1	1/1/14/20	14/31/109/115	-
15	CLA	X	103	12	1/1/13/20	3/25/103/115	-
15	CLA	B	830	2	1/1/15/20	12/37/115/115	-
15	CLA	O	817	2	1/1/15/20	9/37/115/115	-
15	CLA	N	807	1	1/1/15/20	18/37/115/115	-
15	CLA	a	835	1	1/1/15/20	9/37/115/115	-
18	BCR	a	850	-	-	13/29/63/63	0/2/2/2
15	CLA	O	802	24	1/1/15/20	14/37/115/115	-
15	CLA	O	822	24	1/1/12/20	9/23/101/115	-
18	BCR	B	844	-	-	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BCR	O	849	-	-	5/29/63/63	0/2/2/2
19	LHG	A	851	-	-	13/46/46/53	-
15	CLA	A	818	1	1/1/15/20	20/37/115/115	-
21	LMG	T	103	-	-	13/32/52/70	0/1/1/1
15	CLA	B	807	2	1/1/15/20	11/37/115/115	-
15	CLA	O	808	2	1/1/15/20	7/37/115/115	-
15	CLA	O	831	2	1/1/15/20	15/37/115/115	-
15	CLA	a	818	1	1/1/15/20	20/37/115/115	-
15	CLA	a	834	1	1/1/15/20	6/37/115/115	-
19	LHG	X	102	-	-	21/53/53/53	-
15	CLA	B	802	-	1/1/15/20	9/37/115/115	-
15	CLA	b	832	2	1/1/15/20	10/37/115/115	-
18	BCR	g	102	-	-	5/29/63/63	0/2/2/2
15	CLA	B	835	2	1/1/15/20	10/37/115/115	-
15	CLA	A	822	24	1/1/15/20	15/37/115/115	-
15	CLA	b	838	2	1/1/15/20	13/37/115/115	-
15	CLA	b	837	2	1/1/15/20	10/37/115/115	-
19	LHG	L	207	-	-	16/53/53/53	-
15	CLA	A	810	1	1/1/13/20	10/28/106/115	-
15	CLA	N	818	1	1/1/15/20	20/37/115/115	-
15	CLA	A	833	1	1/1/13/20	4/25/103/115	-
15	CLA	a	803	-	1/1/15/20	12/37/115/115	-
20	LMT	a	853	-	-	10/14/54/61	0/2/2/2
18	BCR	k	102	-	-	7/29/63/63	0/2/2/2
18	BCR	A	848	-	-	6/29/63/63	0/2/2/2
15	CLA	b	825	24	1/1/15/20	14/37/115/115	-
18	BCR	S	202	-	-	2/29/63/63	0/2/2/2
15	CLA	b	824	24	1/1/15/20	9/37/115/115	-
13	CL0	A	801	1	3/3/20/25	7/37/135/135	-
15	CLA	a	842	1	1/1/15/20	10/37/115/115	-
18	BCR	I	101	-	-	10/29/63/63	0/2/2/2
15	CLA	b	806	2	1/1/15/20	16/37/115/115	-
15	CLA	A	838	1	1/1/13/20	11/25/103/115	-
15	CLA	A	807	1	1/1/15/20	18/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	LHG	k	101	-	-	17/53/53/53	-
15	CLA	B	829	2	1/1/15/20	14/37/115/115	-
15	CLA	N	833	1	1/1/13/20	3/25/103/115	-
15	CLA	B	811	2	-	10/27/105/115	-
17	SF4	a	844	1,2	-	-	0/6/5/5
15	CLA	O	841	2	1/1/15/20	13/37/115/115	-
15	CLA	A	820	1	1/1/15/20	20/37/115/115	-
15	CLA	B	839	2	1/1/15/20	13/37/115/115	-
14	F6C	O	833	2	-	5/41/97/97	-
15	CLA	B	826	2	1/1/15/20	8/37/115/115	-
14	F6C	N	856	24	-	17/41/97/97	-
19	LHG	l	101	-	-	24/48/48/53	-
15	CLA	a	839	1	1/1/15/20	14/37/115/115	-
15	CLA	O	821	2	1/1/11/20	5/13/91/115	-
15	CLA	B	823	24	1/1/15/20	15/37/115/115	-
20	LMT	A	852	-	-	2/17/57/61	0/2/2/2
21	LMG	a	855	-	-	8/39/59/70	0/1/1/1
15	CLA	O	807	2	1/1/15/20	5/37/115/115	-
14	F6C	L	204	24	-	12/41/97/97	-
15	CLA	a	823	1	1/1/13/20	8/27/105/115	-
15	CLA	O	804	2	1/1/15/20	8/37/115/115	-
15	CLA	N	820	1	1/1/15/20	20/37/115/115	-
18	BCR	i	101	-	-	0/18/35/63	0/1/1/2
15	CLA	a	829	1	1/1/14/20	17/31/109/115	-
14	F6C	a	856	24	-	18/41/97/97	-
15	CLA	b	809	2	1/1/15/20	15/37/115/115	-
21	LMG	h	102	-	-	16/50/70/70	0/1/1/1
15	CLA	b	826	2	1/1/15/20	5/37/115/115	-
15	CLA	b	807	2	1/1/15/20	3/37/115/115	-
15	CLA	B	816	2	1/1/14/20	14/31/109/115	-
15	CLA	b	814	2	1/1/15/20	15/37/115/115	-
18	BCR	f	203	-	-	2/29/63/63	0/2/2/2
15	CLA	b	820	2	1/1/13/20	11/25/103/115	-
15	CLA	a	816	1	1/1/11/20	8/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	N	829	1	1/1/14/20	17/31/109/115	-
15	CLA	B	803	2	1/1/15/20	8/37/115/115	-
14	F6C	N	802	24	-	7/41/97/97	-
15	CLA	Z	103	12	1/1/13/20	5/25/103/115	-
18	BCR	h	101	-	-	7/29/63/63	0/2/2/2
20	LMT	N	853	-	-	9/14/54/61	0/2/2/2
15	CLA	B	832	2	1/1/13/20	8/25/103/115	-
15	CLA	b	811	2	1/1/15/20	11/37/115/115	-
15	CLA	O	823	2	1/1/13/20	11/25/103/115	-
18	BCR	a	848	-	-	7/29/63/63	0/2/2/2
15	CLA	A	837	1	1/1/12/20	10/21/99/115	-
15	CLA	L	203	10	1/1/14/20	12/31/109/115	-
15	CLA	B	837	2	1/1/15/20	12/37/115/115	-
15	CLA	b	819	24	1/1/15/20	9/37/115/115	-
15	CLA	A	840	1	1/1/12/20	2/19/97/115	-
15	CLA	O	812	2	1/1/11/20	3/13/91/115	-
18	BCR	N	850	-	-	13/29/63/63	0/2/2/2
15	CLA	a	813	1	1/1/12/20	6/24/102/115	-
18	BCR	a	847	-	-	6/29/63/63	0/2/2/2
14	F6C	a	802	24	-	7/41/97/97	-
15	CLA	N	836	1	1/1/12/20	9/24/102/115	-
21	LMG	O	850	-	-	7/50/70/70	0/1/1/1
15	CLA	O	828	2	1/1/15/20	7/37/115/115	-
15	CLA	B	819	2	1/1/11/20	5/13/91/115	-
18	BCR	B	846	-	-	4/29/63/63	0/2/2/2
15	CLA	a	841	1	1/1/15/20	14/37/115/115	-
18	BCR	N	847	-	-	6/29/63/63	0/2/2/2
15	CLA	f	201	24	1/1/15/20	8/37/115/115	-
18	BCR	K	101	-	-	0/18/35/63	0/1/1/2
15	CLA	B	818	2	1/1/13/20	9/25/103/115	-
15	CLA	A	842	1	1/1/15/20	9/37/115/115	-
15	CLA	B	834	24	1/1/11/20	10/13/91/115	-
15	CLA	F	201	24	1/1/15/20	8/37/115/115	-
16	PQN	N	843	-	-	1/23/43/43	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	LMG	W	1505	-	-	11/45/65/70	0/1/1/1
15	CLA	O	824	24	1/1/15/20	11/37/115/115	-
21	LMG	L	206	-	-	12/45/65/70	0/1/1/1
18	BCR	B	843	-	-	4/29/63/63	0/2/2/2
18	BCR	b	846	-	-	7/29/63/63	0/2/2/2
19	LHG	N	851	-	-	13/46/46/53	-
18	BCR	O	846	-	-	8/29/63/63	0/2/2/2
15	CLA	a	805	1,15	1/1/14/20	9/31/109/115	-
15	CLA	b	818	2	1/1/14/20	12/31/109/115	-
15	CLA	b	801	2	1/1/15/20	11/37/115/115	-
14	F6C	A	824	24	-	9/25/81/97	-
18	BCR	B	841	-	-	3/29/63/63	0/2/2/2
20	LMT	a	852	-	-	1/17/57/61	0/2/2/2
15	CLA	W	1501	10	1/1/15/20	8/37/115/115	-
14	F6C	A	826	24	-	15/41/97/97	-
15	CLA	a	836	1	1/1/12/20	7/24/102/115	-
19	LHG	W	1506	-	-	16/53/53/53	-
18	BCR	a	849	-	-	3/29/63/63	0/2/2/2
15	CLA	N	812	1,15	1/1/15/20	19/37/115/115	-
15	CLA	O	819	24	1/1/15/20	8/37/115/115	-
14	F6C	W	1503	24	-	14/41/97/97	-
15	CLA	K	103	24	1/1/12/20	3/19/97/115	-
18	BCR	N	846	-	-	8/29/63/63	0/2/2/2
15	CLA	a	808	1	1/1/11/20	1/13/91/115	-
22	LFA	j	208	-	-	0/12/12/17	-
15	CLA	a	831	1	1/1/15/20	11/37/115/115	-
15	CLA	a	833	1	1/1/13/20	3/25/103/115	-
15	CLA	A	809	1	1/1/14/20	11/31/109/115	-
18	BCR	O	848	-	-	6/29/63/63	0/2/2/2
15	CLA	a	821	1	1/1/14/20	8/31/109/115	-
15	CLA	A	804	1	1/1/15/20	6/37/115/115	-
18	BCR	g	101	-	-	7/29/63/63	0/2/2/2
18	BCR	A	846	-	-	8/29/63/63	0/2/2/2
15	CLA	O	803	-	1/1/15/20	8/37/115/115	-
15	CLA	l	103	12	1/1/13/20	2/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	N	810	1	1/1/13/20	9/28/106/115	-
17	SF4	c	102	3	-	-	0/6/5/5
15	CLA	O	832	2	1/1/15/20	11/37/115/115	-
16	PQN	a	843	-	-	0/23/43/43	0/2/2/2
18	BCR	j	205	-	-	4/29/63/63	0/2/2/2
19	LHG	a	851	-	-	13/46/46/53	-
18	BCR	W	1504	-	-	4/29/63/63	0/2/2/2
15	CLA	O	827	2	1/1/14/20	15/34/112/115	-
15	CLA	b	835	24	1/1/11/20	4/13/91/115	-
15	CLA	B	812	2	1/1/15/20	15/37/115/115	-
18	BCR	O	845	-	-	4/29/63/63	0/2/2/2
15	CLA	N	804	1	1/1/15/20	6/37/115/115	-
15	CLA	O	806	2	1/1/15/20	16/37/115/115	-
18	BCR	j	201	-	-	5/29/63/63	0/2/2/2
19	LHG	X	101	-	-	22/48/48/53	-
15	CLA	N	822	24	1/1/15/20	17/37/115/115	-
15	CLA	b	834	2	1/1/13/20	8/25/103/115	-
18	BCR	N	849	-	-	3/29/63/63	0/2/2/2
18	BCR	O	843	-	-	3/29/63/63	0/2/2/2
15	CLA	A	825	1	1/1/15/20	6/37/115/115	-
15	CLA	N	837	1	1/1/12/20	10/21/99/115	-
19	LHG	Z	102	-	-	22/53/53/53	-
15	CLA	B	806	2	1/1/15/20	5/37/115/115	-
18	BCR	Y	102	-	-	7/29/63/63	0/2/2/2
15	CLA	N	827	24	1/1/13/20	2/25/103/115	-
15	CLA	N	808	1	1/1/11/20	3/13/91/115	-
15	CLA	N	805	1,15	1/1/14/20	9/31/109/115	-
15	CLA	O	829	2	1/1/15/20	11/37/115/115	-
19	LHG	j	207	-	-	16/53/53/53	-
15	CLA	b	803	-	1/1/15/20	9/37/115/115	-
15	CLA	A	803	-	1/1/15/20	12/37/115/115	-
15	CLA	A	830	1	1/1/15/20	9/37/115/115	-
14	F6C	j	204	24	-	13/41/97/97	-
15	CLA	A	815	1	1/1/13/20	5/25/103/115	-



The worst 5 of 1743 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	826	F6C	C2A-C3A	8.76	1.55	1.36
14	L	201	F6C	C2A-C3A	8.73	1.55	1.36
14	A	826	F6C	C2A-C3A	8.71	1.55	1.36
14	O	810	F6C	C2A-C3A	8.70	1.55	1.36
14	a	826	F6C	C2A-C3A	8.70	1.55	1.36

The worst 5 of 2357 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	O	840	F6C	CAA-C2A-C3A	-10.08	109.11	127.88
14	B	838	F6C	CAA-C2A-C3A	-10.06	109.14	127.88
14	b	840	F6C	CAA-C2A-C3A	-10.02	109.21	127.88
14	L	204	F6C	CAA-C2A-C3A	-10.00	109.25	127.88
14	j	204	F6C	CAA-C2A-C3A	-9.96	109.33	127.88

5 of 252 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	A	801	CL0	ND
13	A	801	CL0	NC
13	A	801	CL0	NA
13	N	801	CL0	ND
13	N	801	CL0	NC

5 of 3603 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	802	F6C	C1B-C2B-CMB-OMB
14	A	802	F6C	C3B-C2B-CMB-OMB
14	A	824	F6C	C4B-C3B-CAB-CBB
14	A	824	F6C	C1B-C2B-CMB-OMB
14	A	824	F6C	C3B-C2B-CMB-OMB

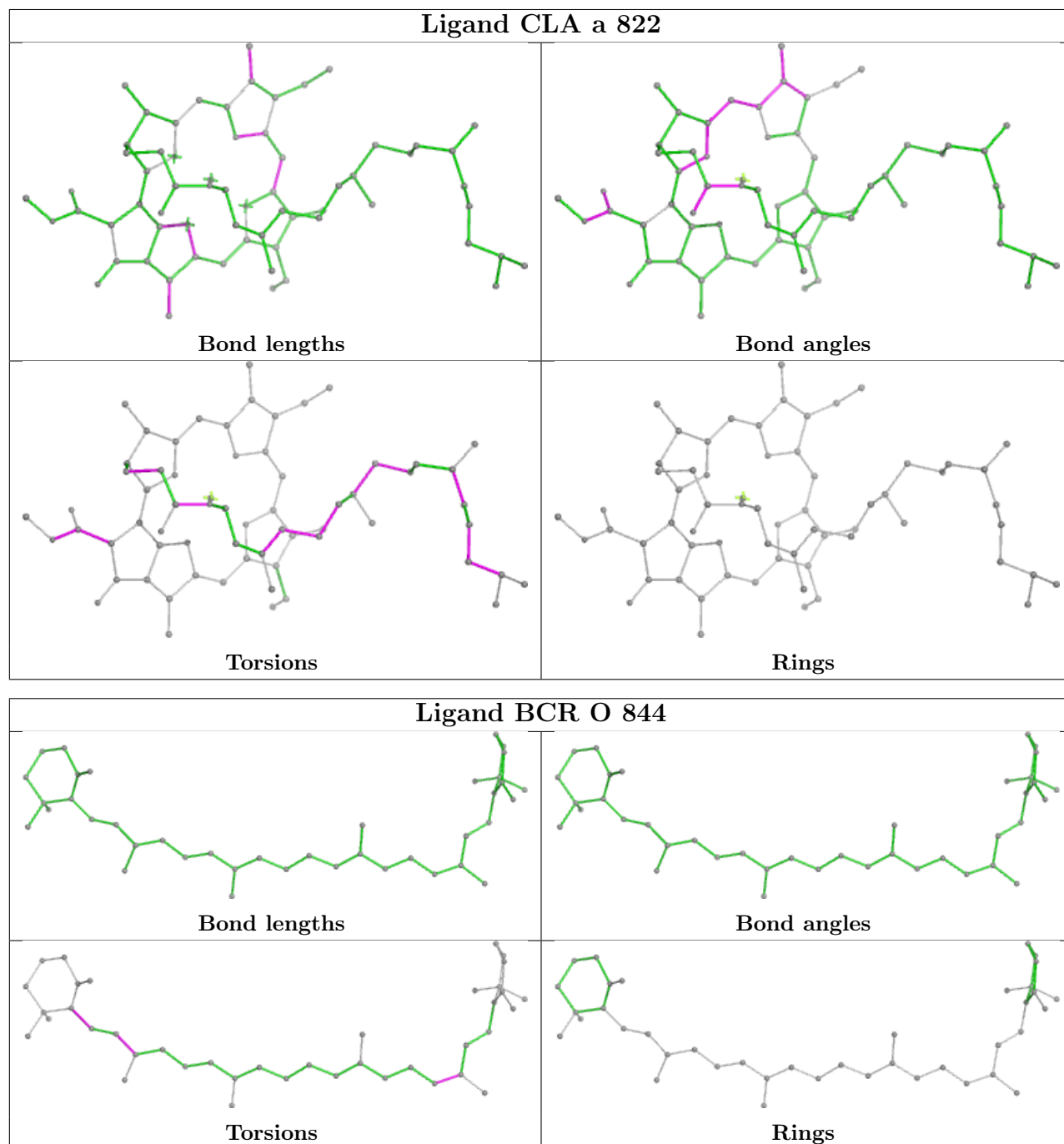
There are no ring outliers.

No monomer is involved in short contacts.

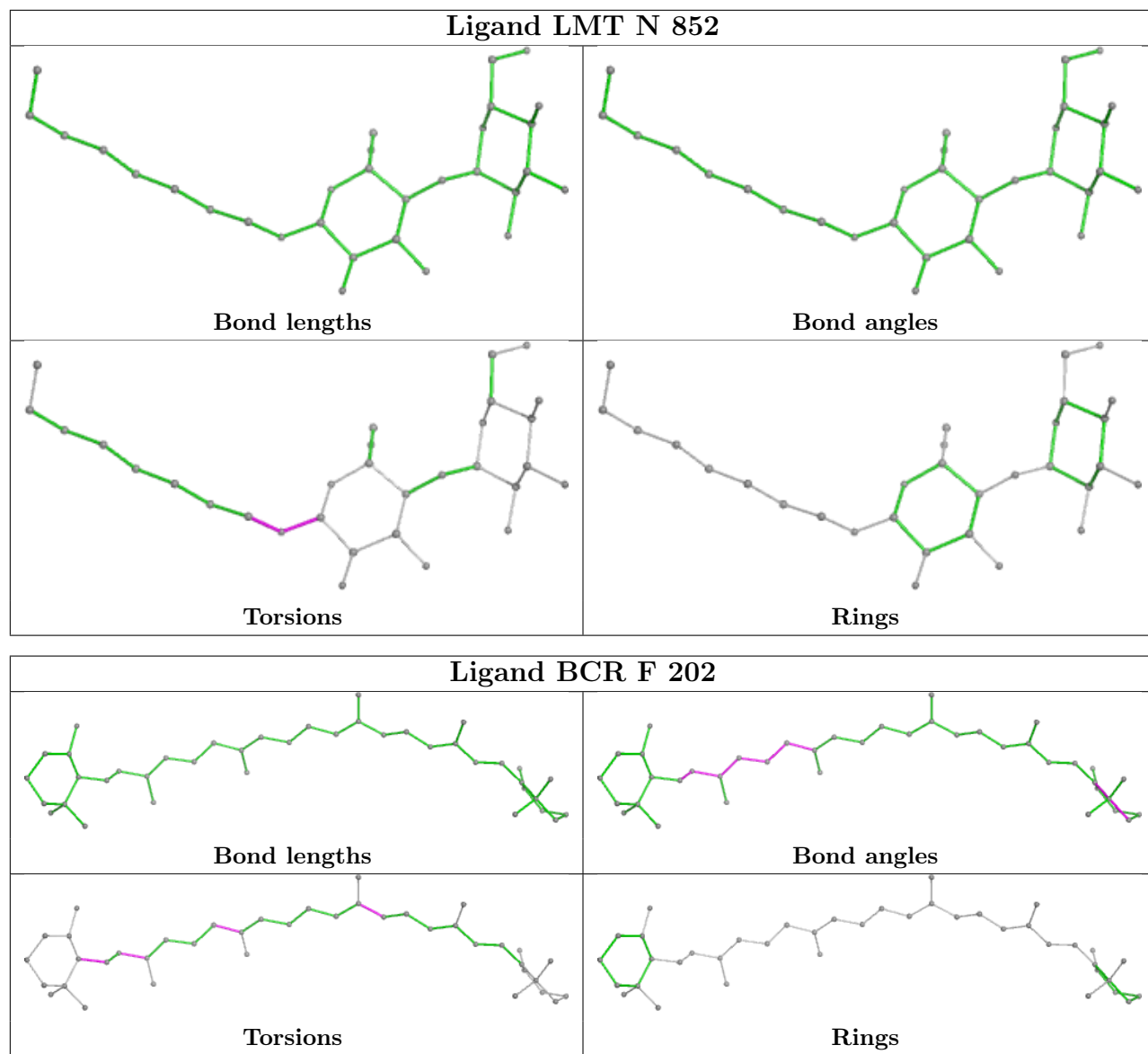
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.



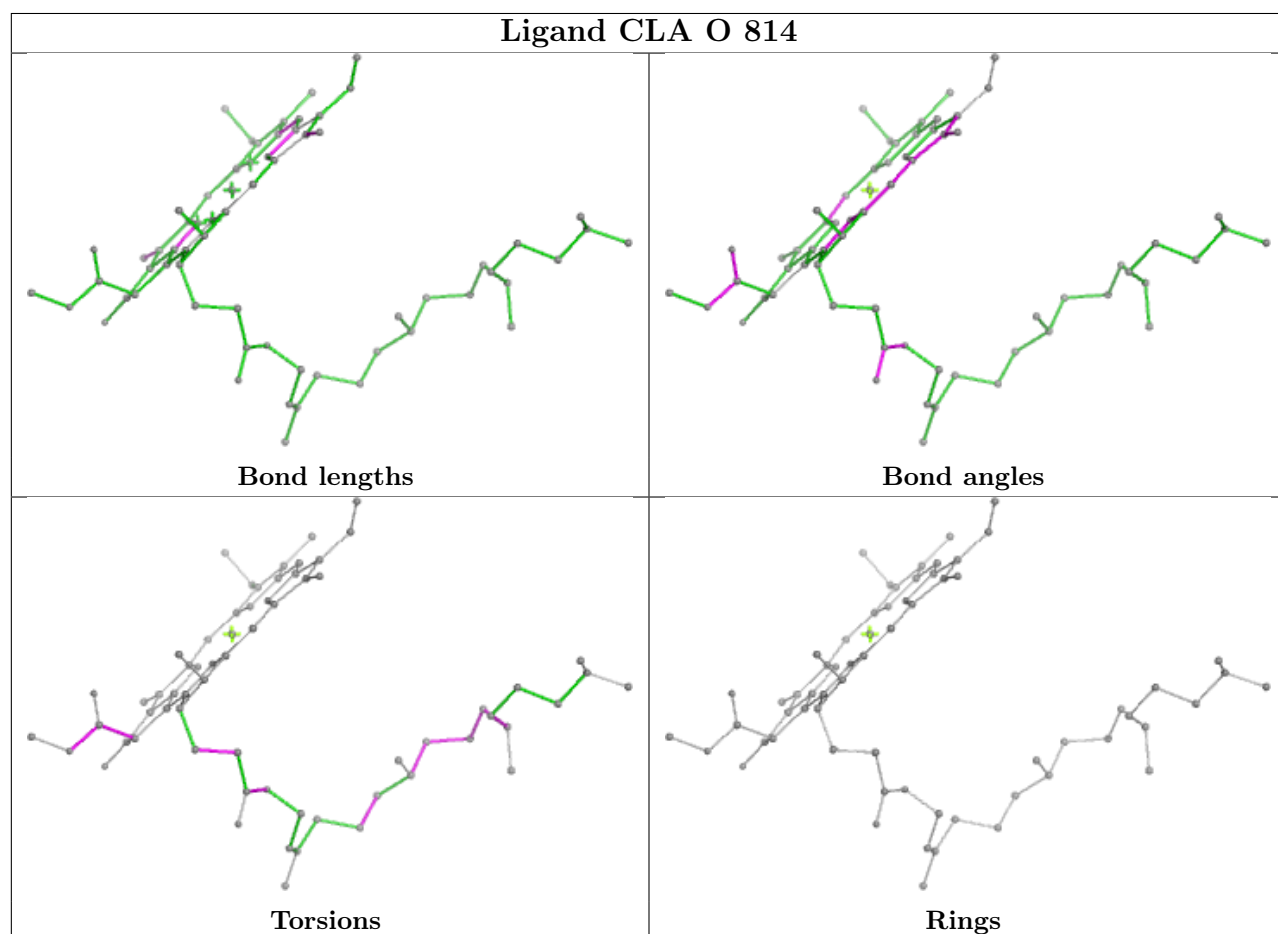
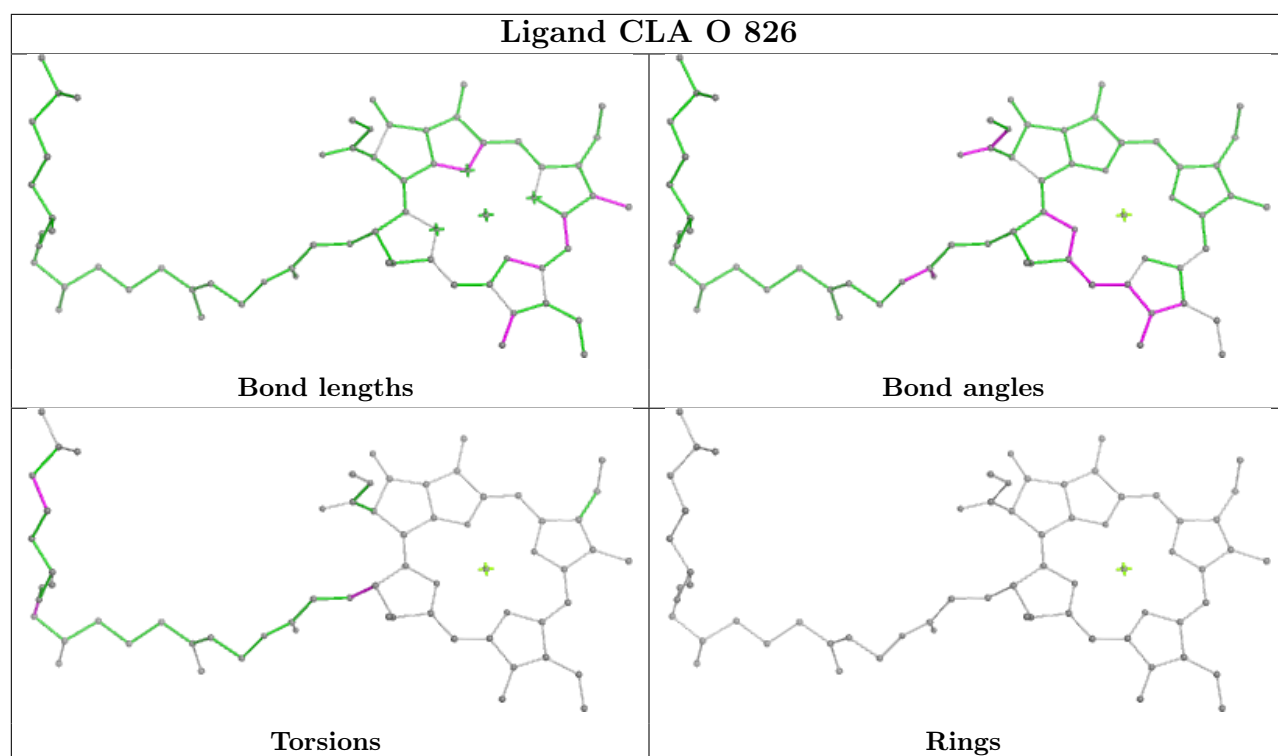
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



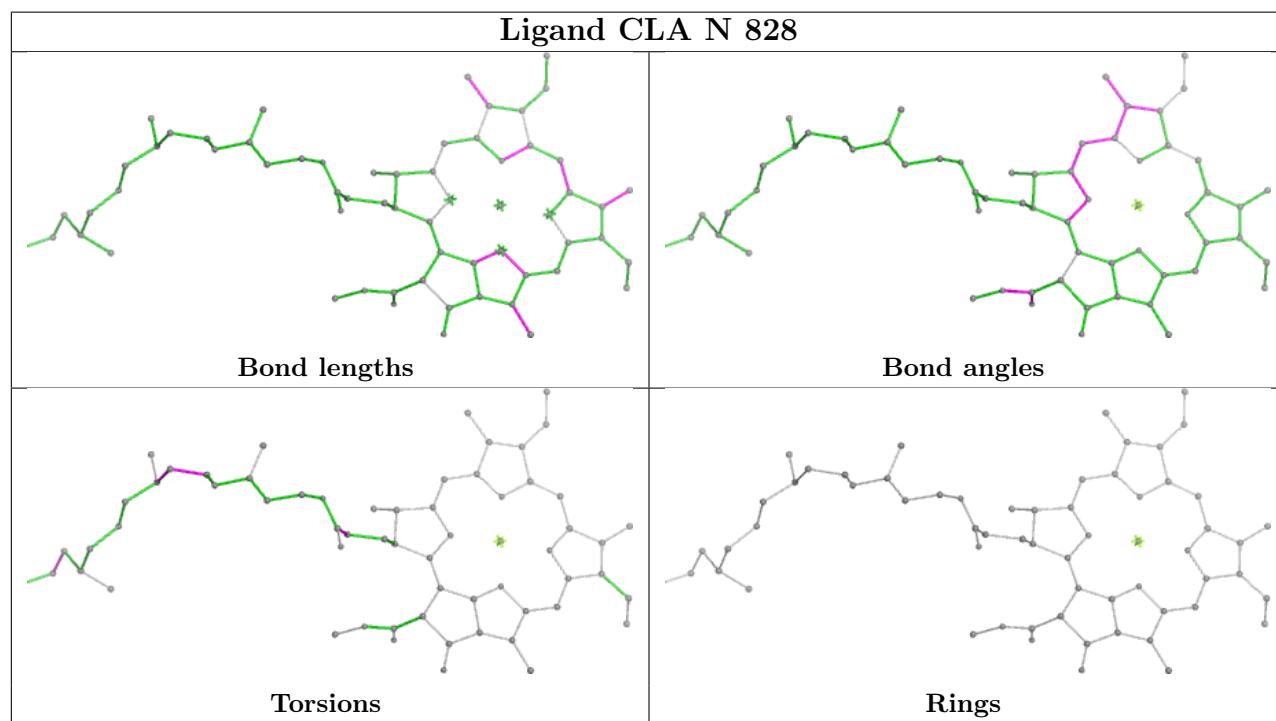
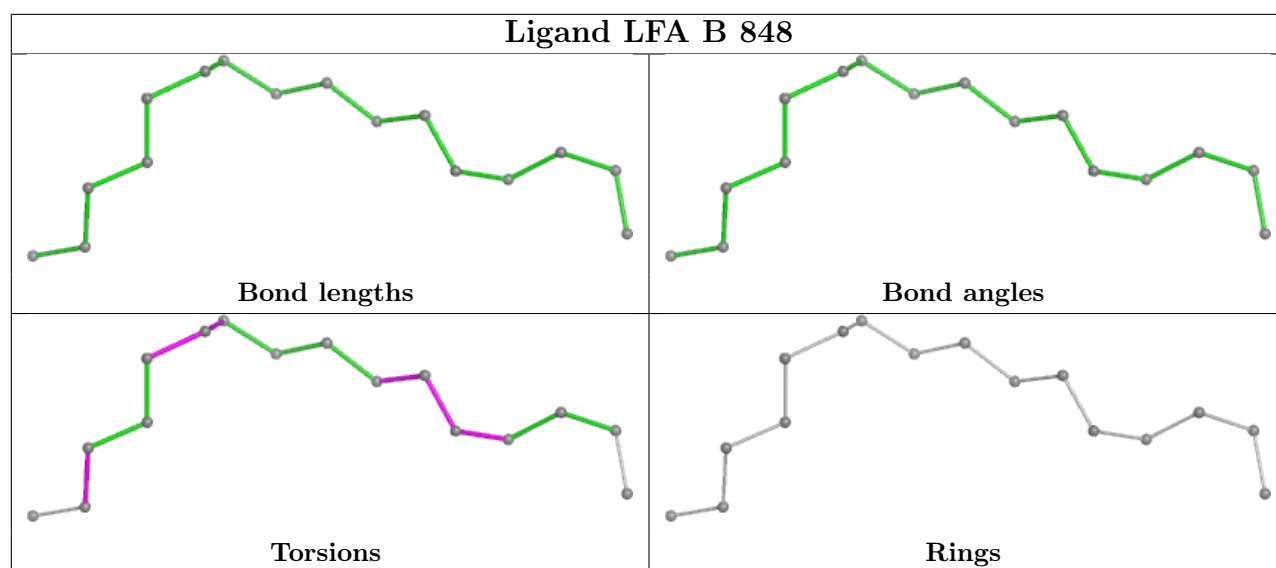




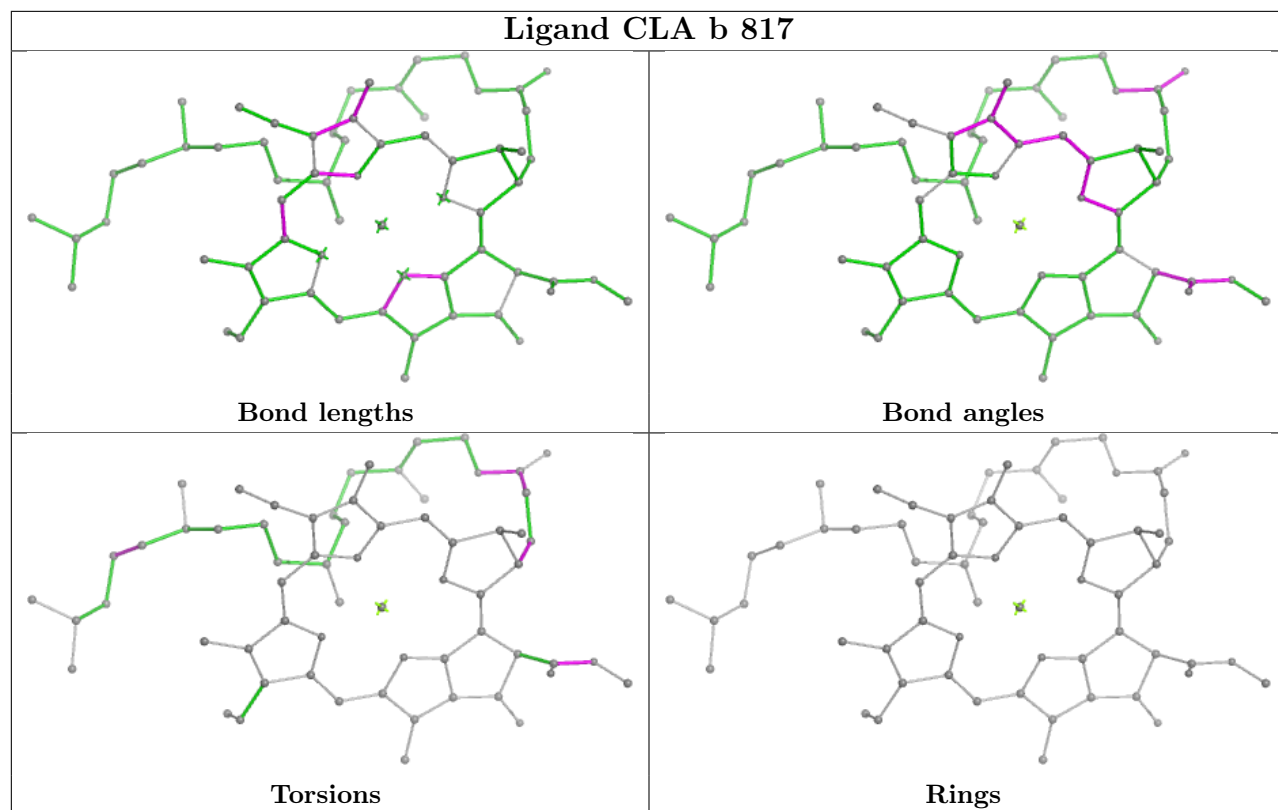




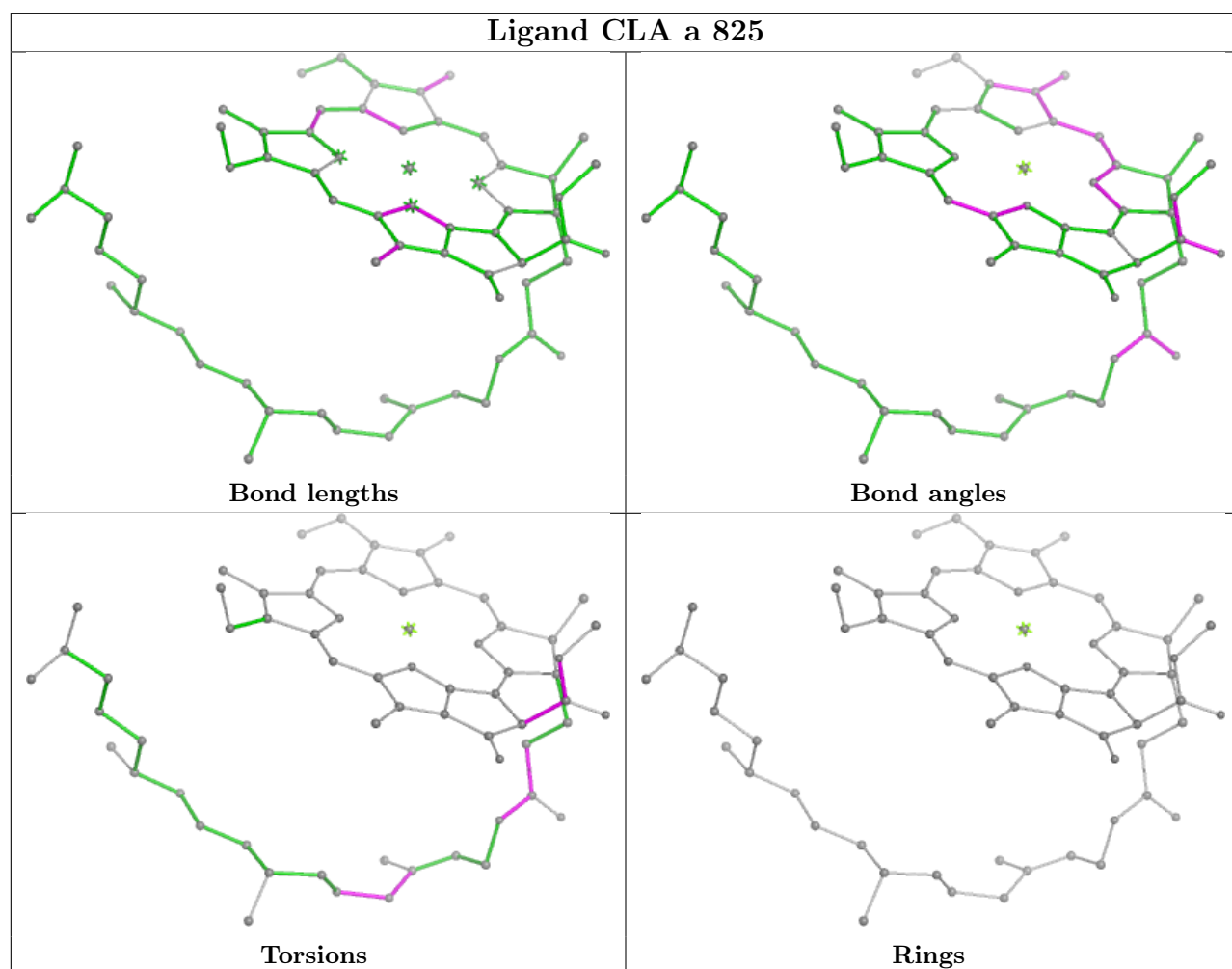






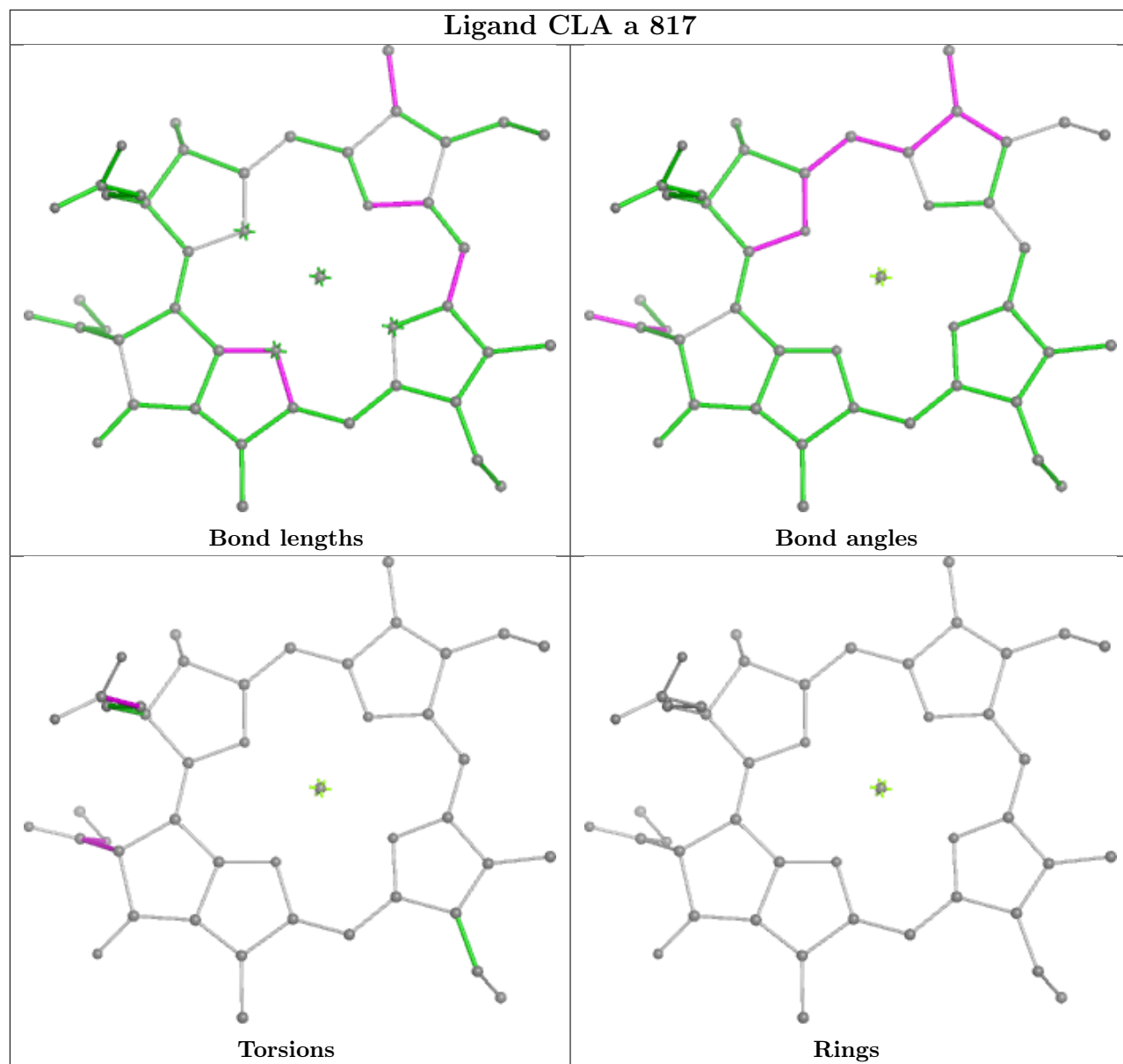






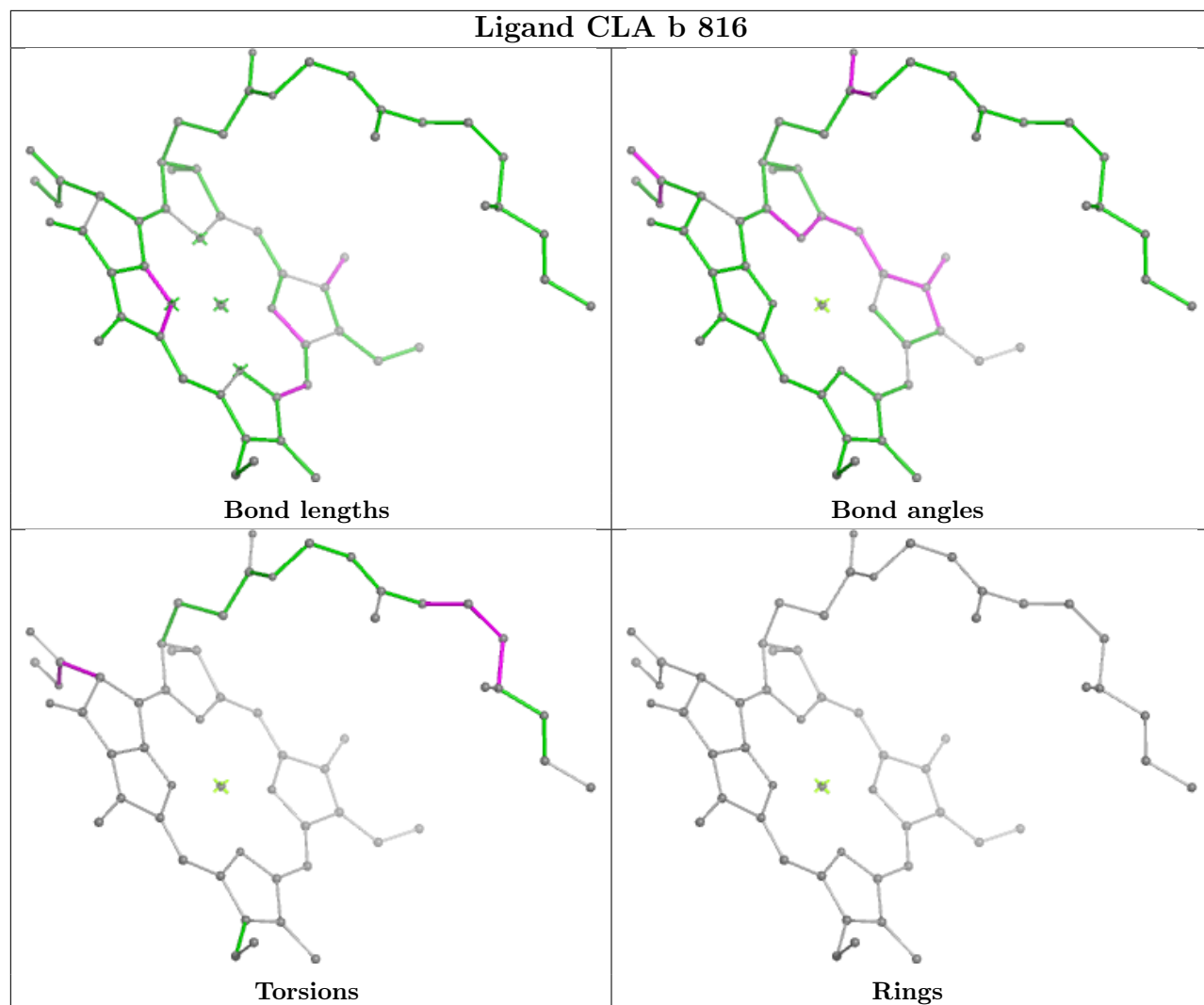


## Ligand CLA a 817

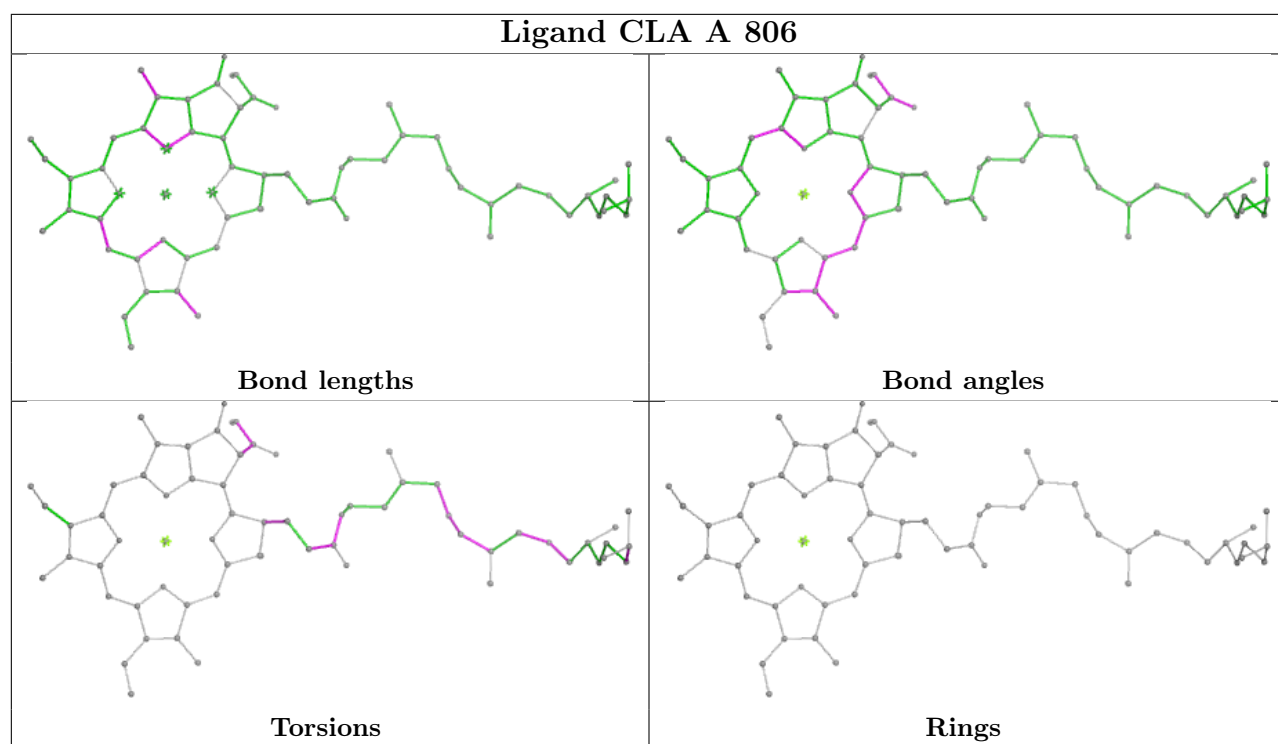




## Ligand CLA b 816

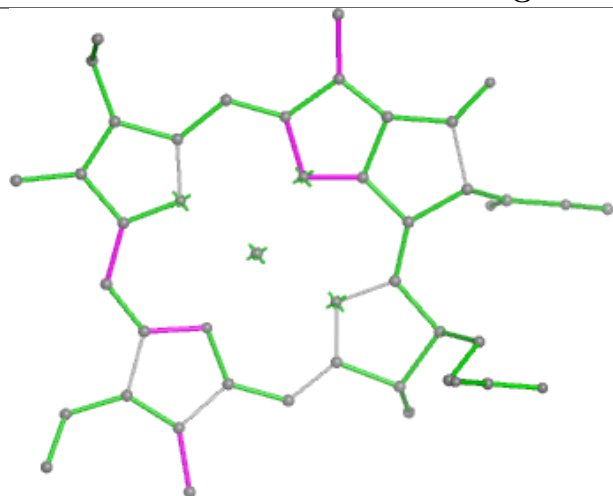




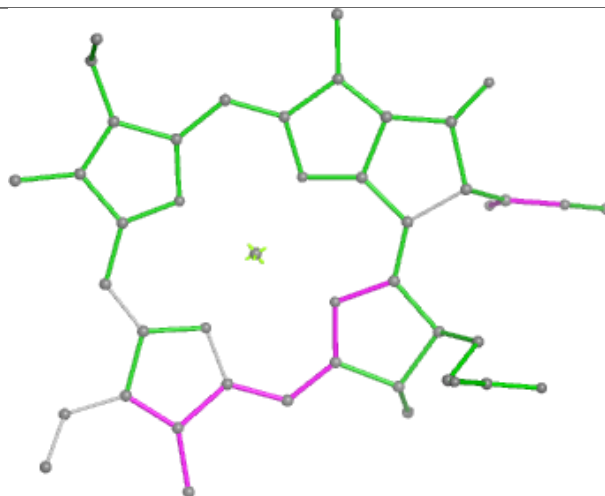




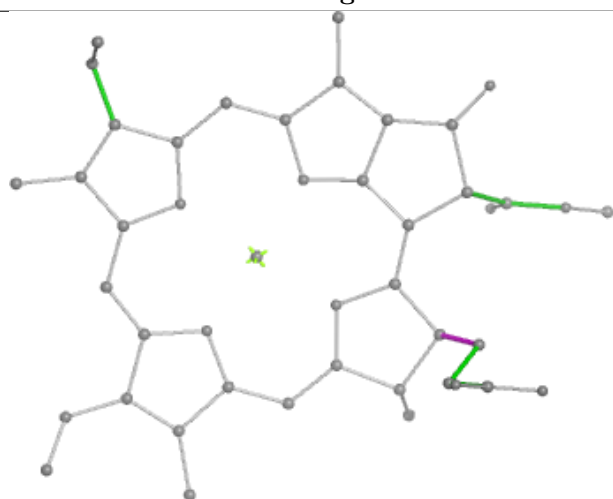
## Ligand CLA O 835



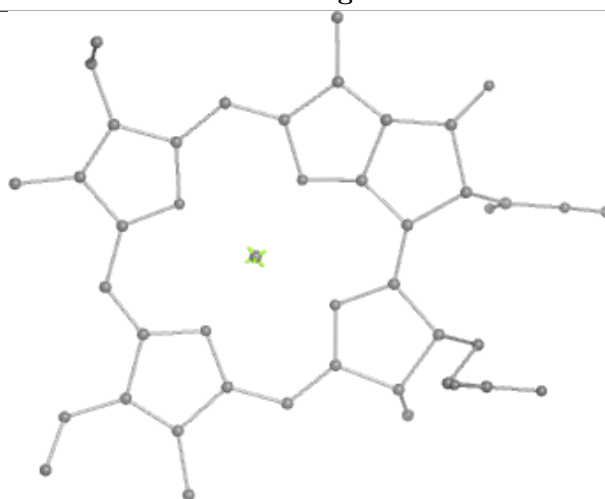
Bond lengths



Bond angles

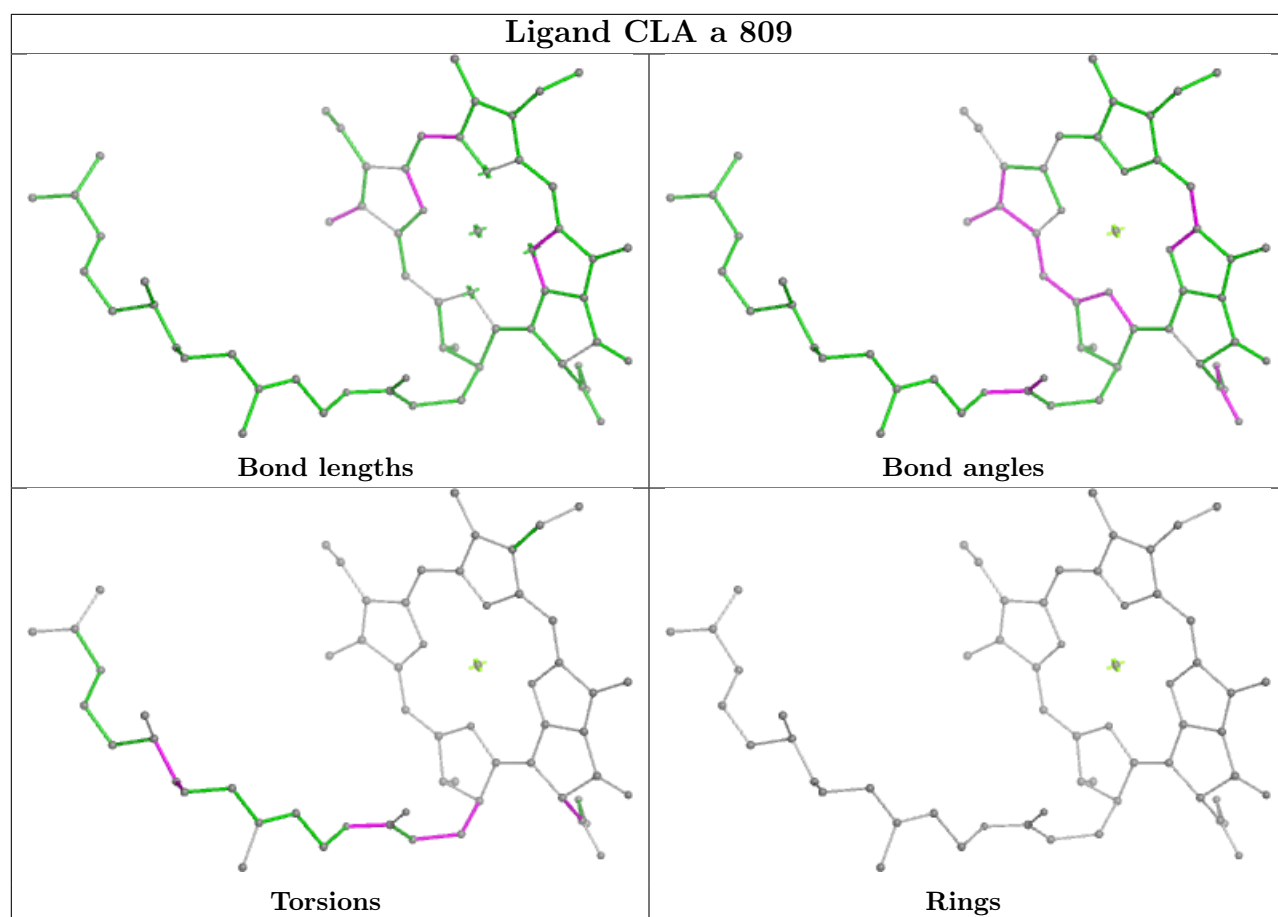


Torsions

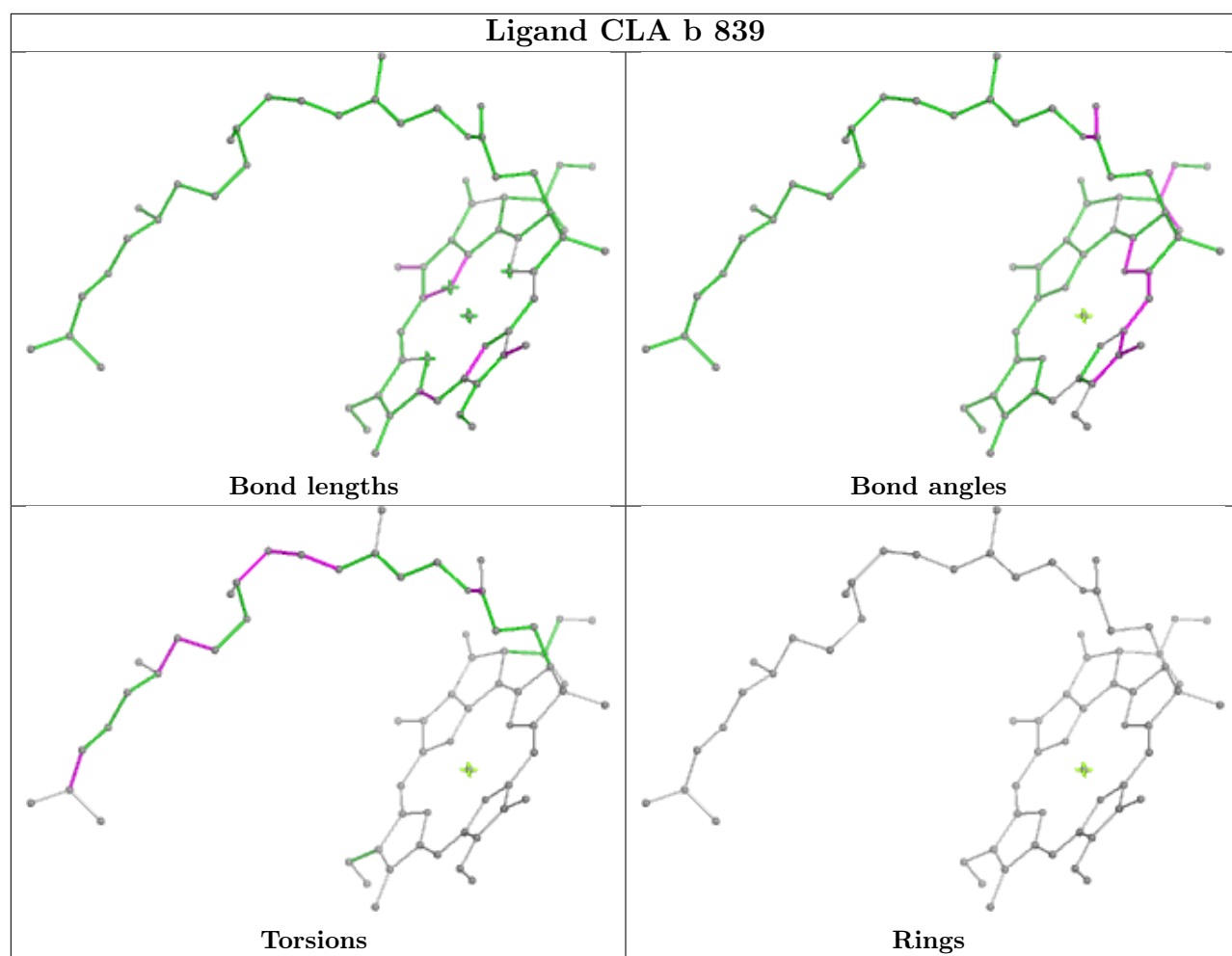


Rings



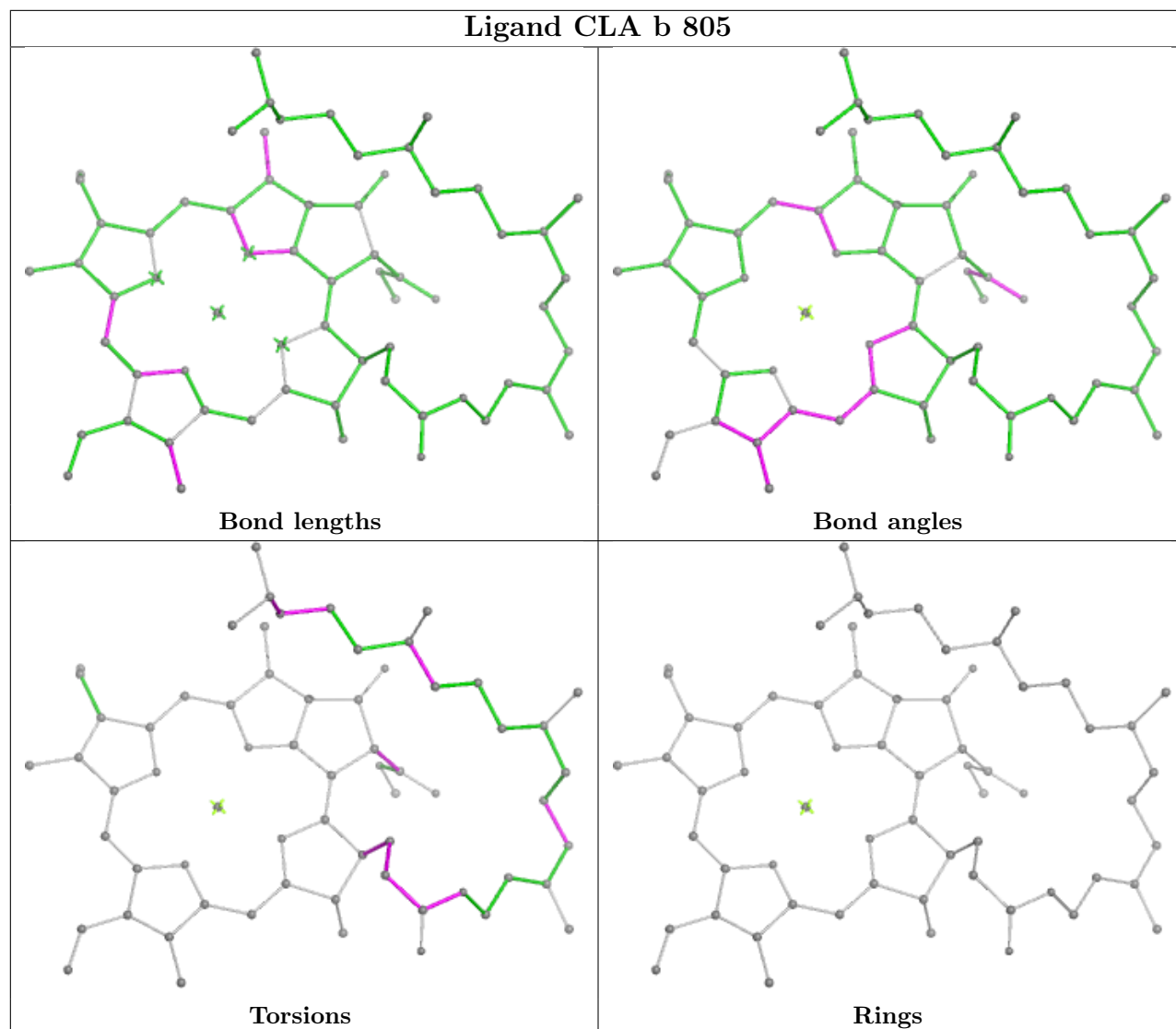




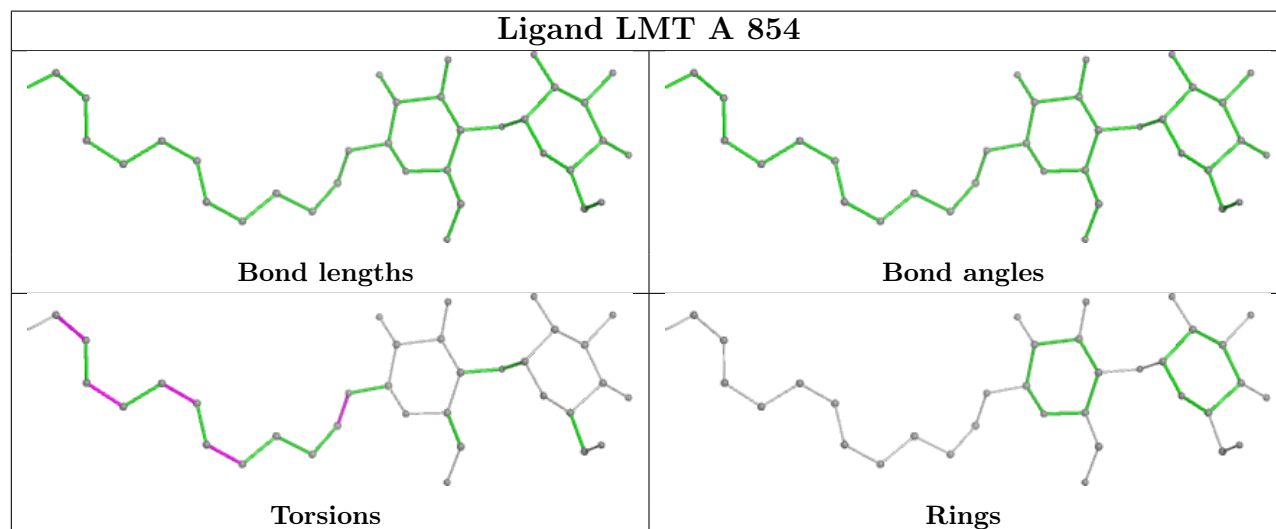




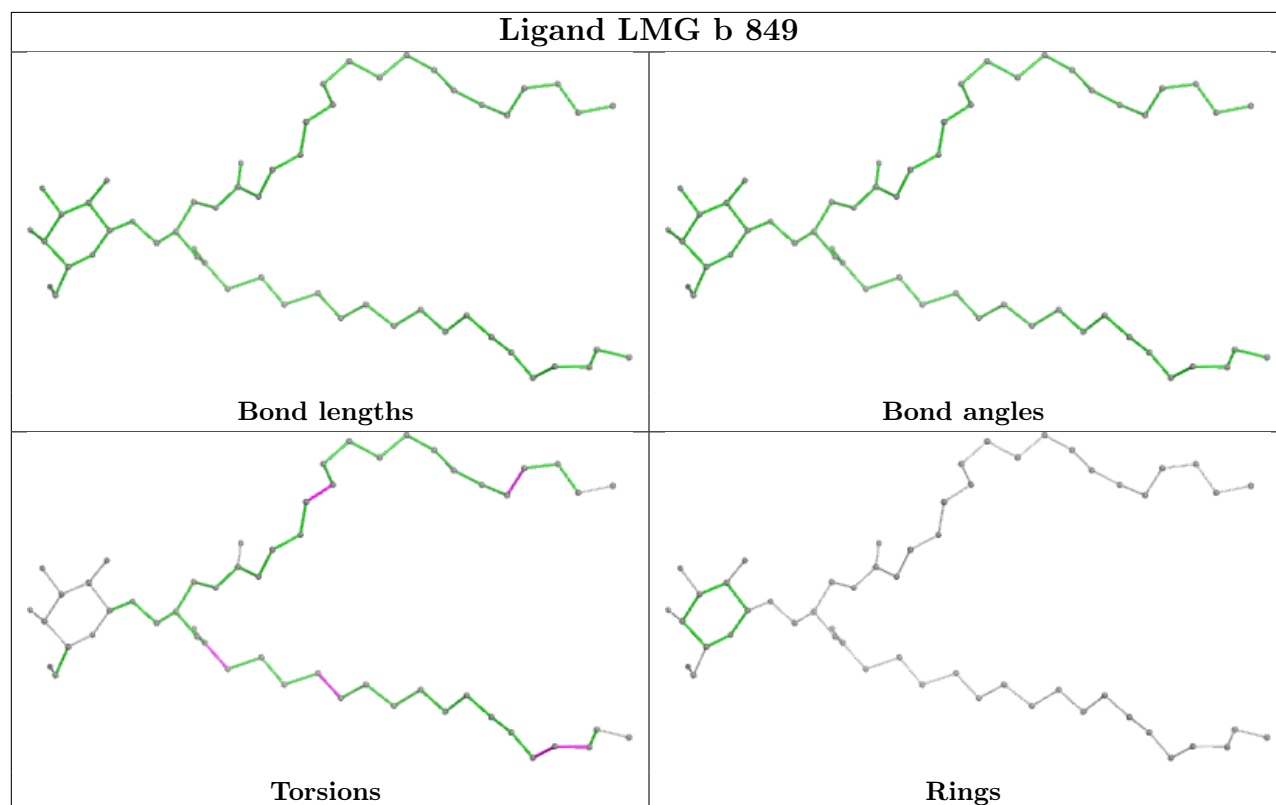
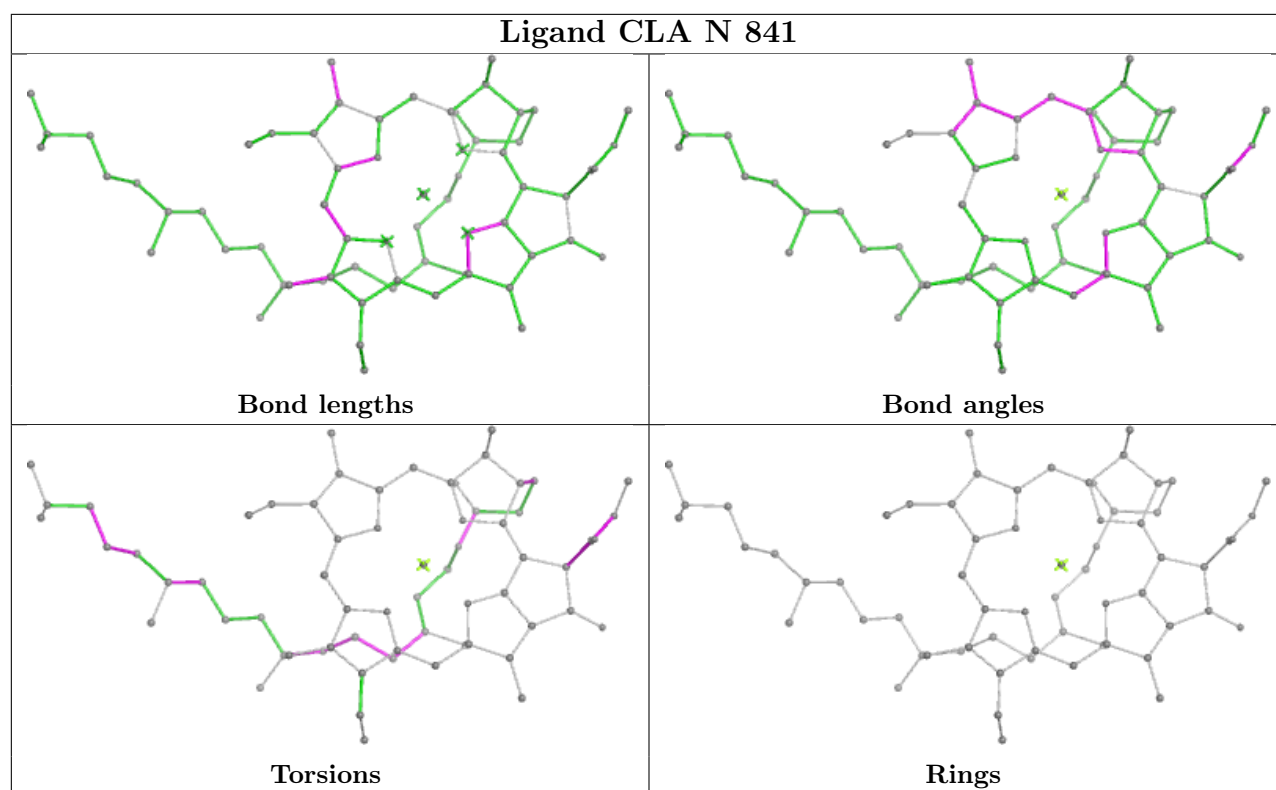
## Ligand CLA b 805



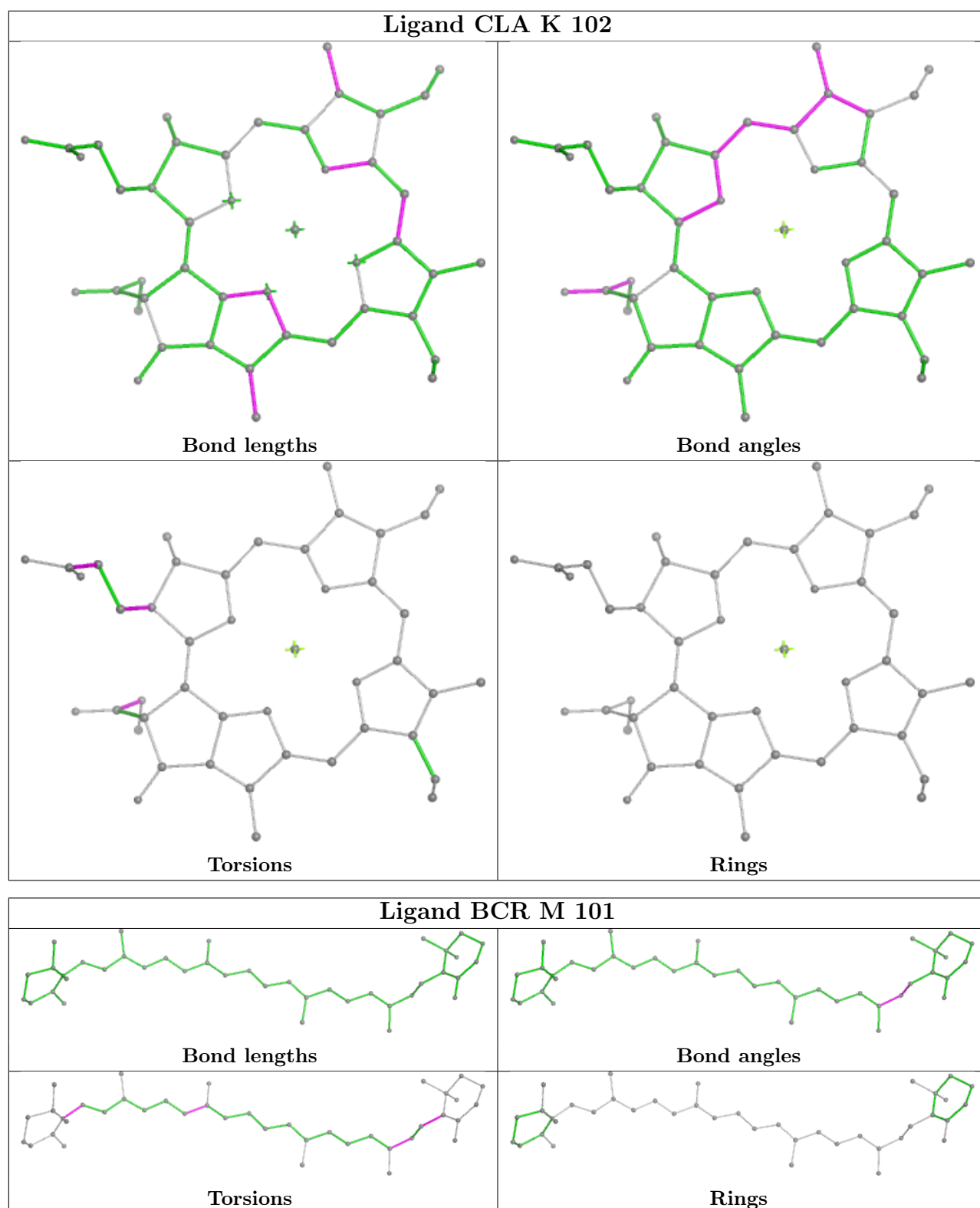
## Ligand LMT A 854





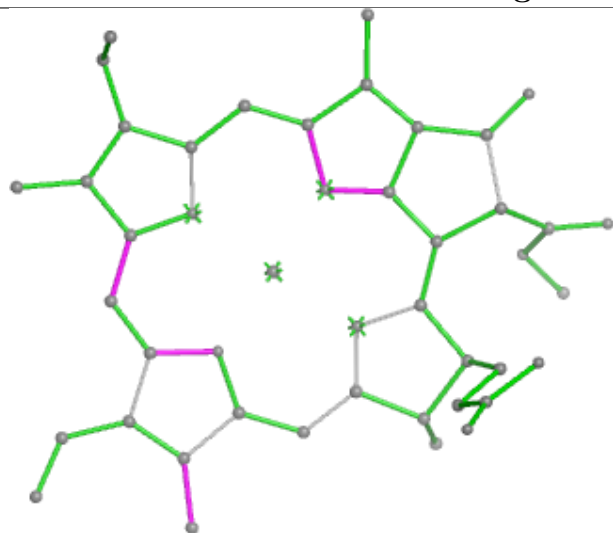




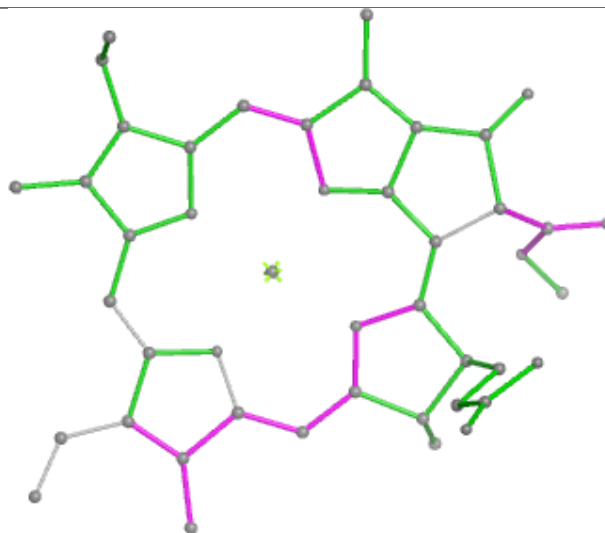




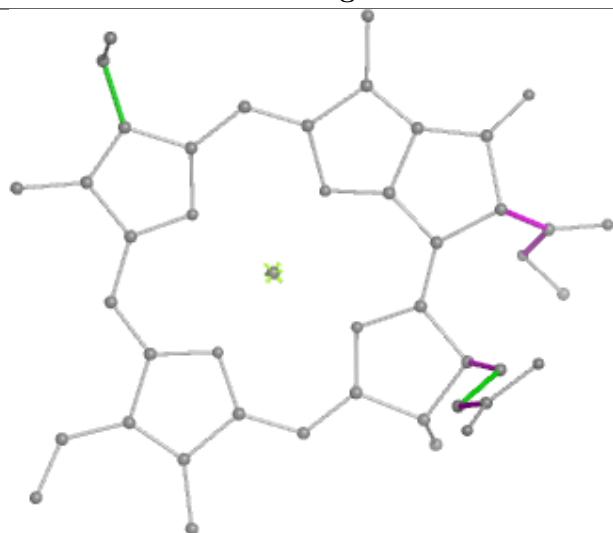
## Ligand CLA O 815



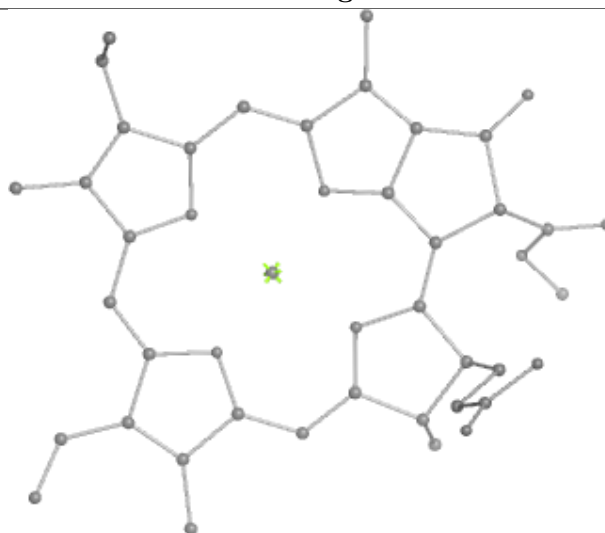
Bond lengths



Bond angles

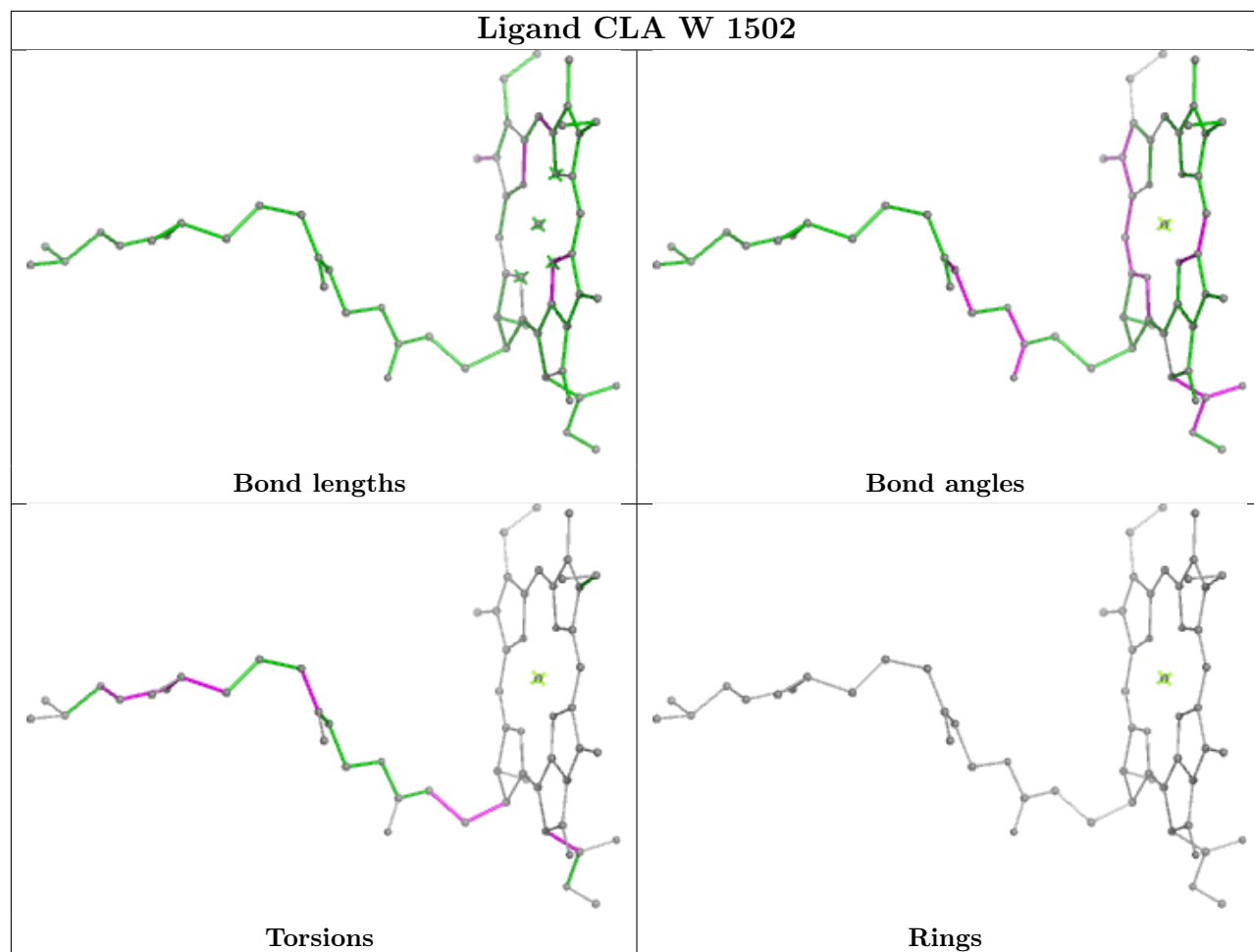


Torsions

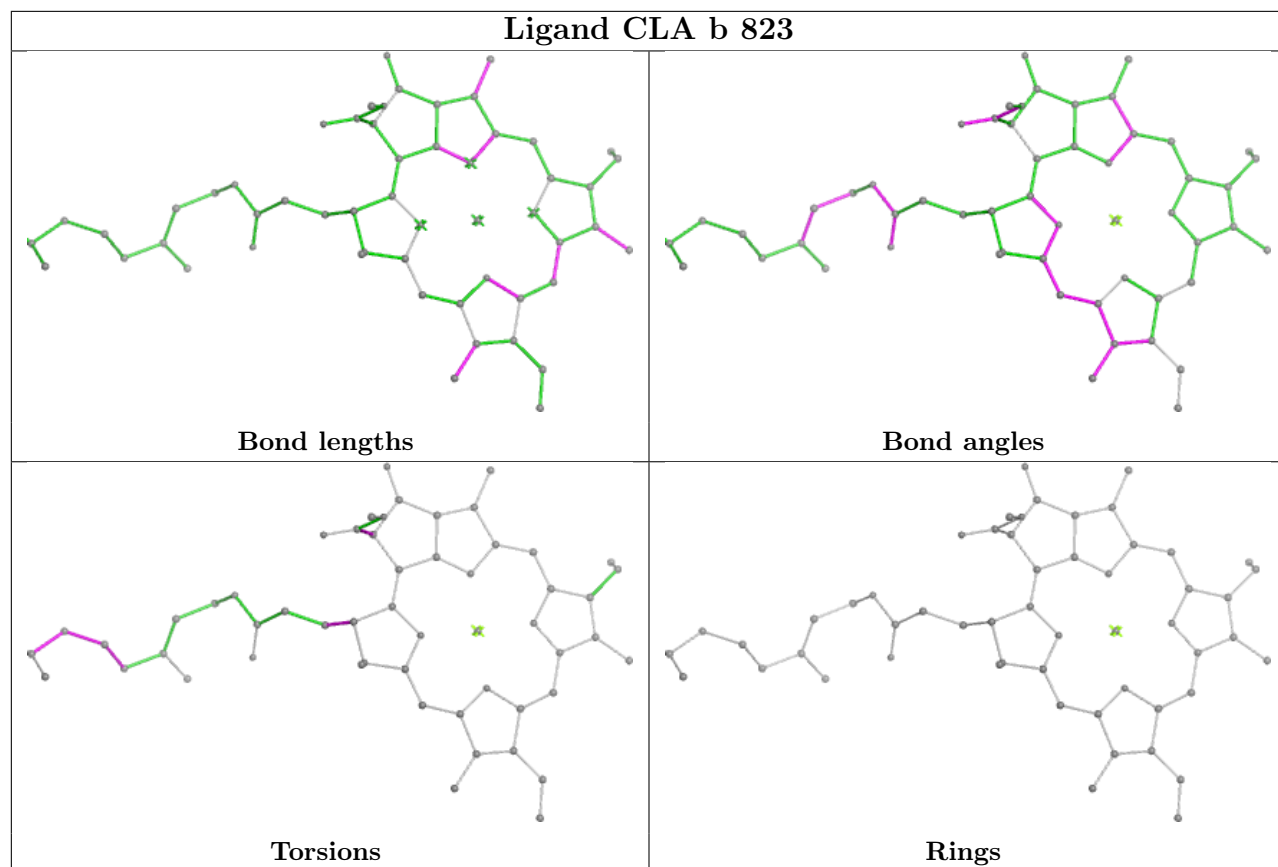


Rings

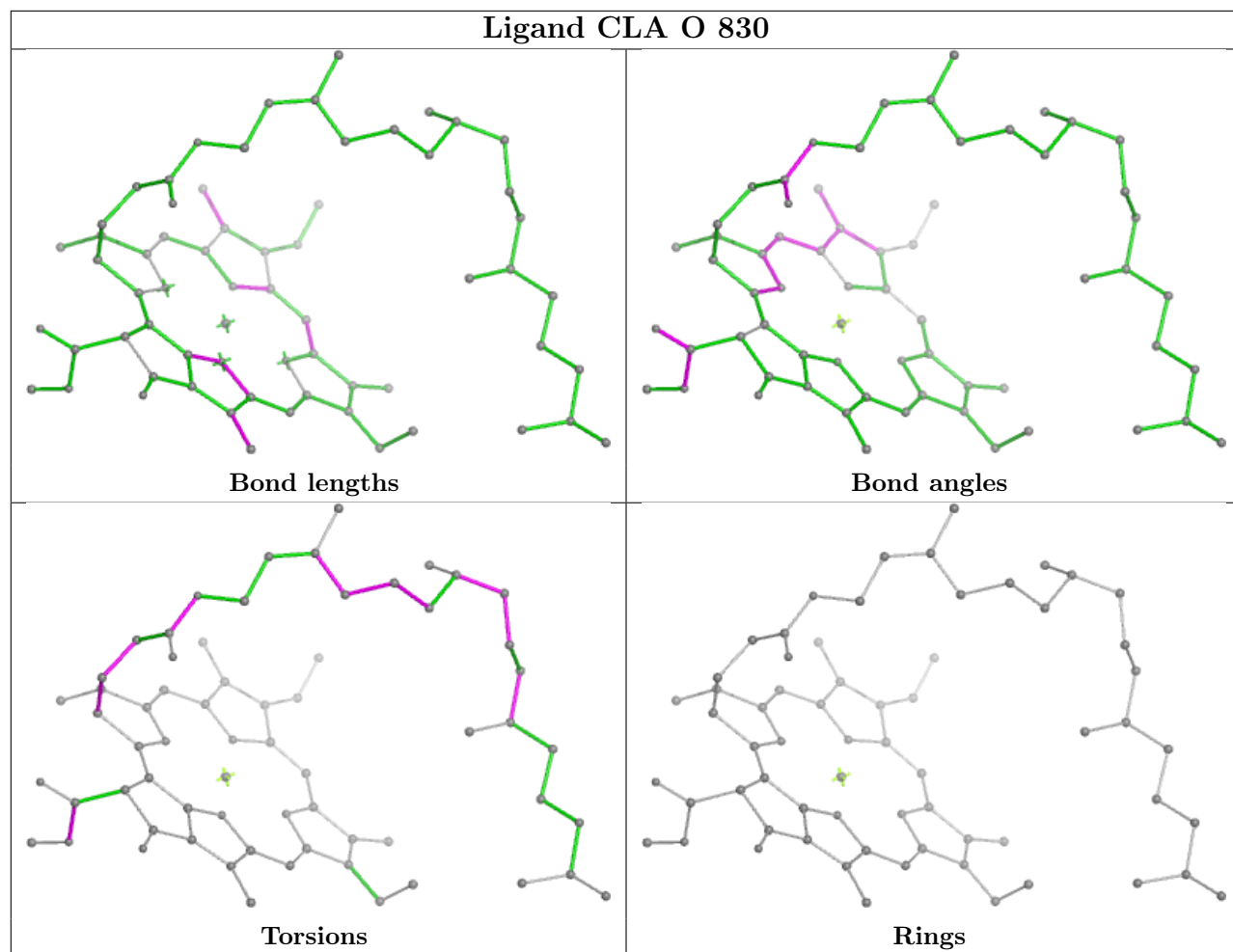






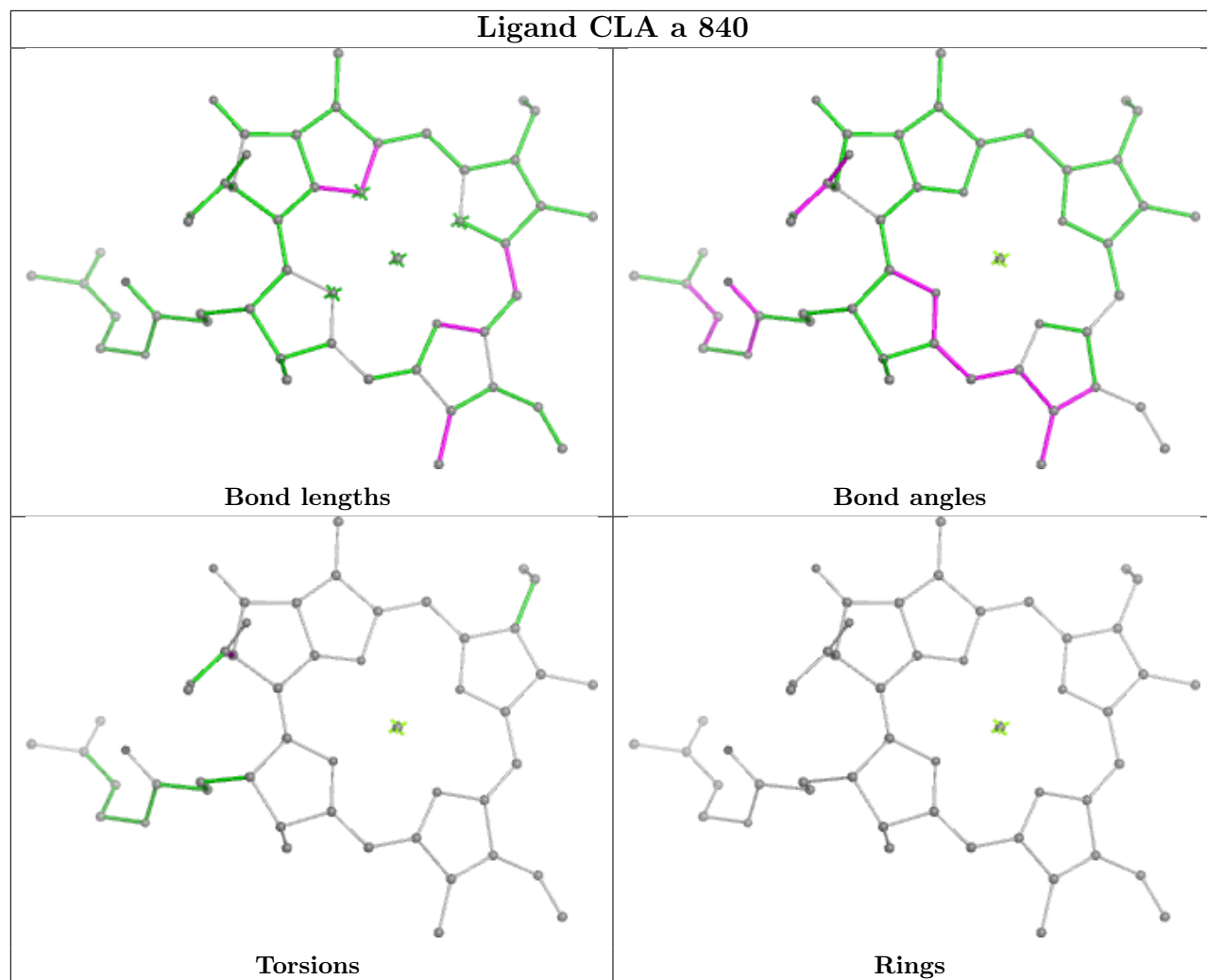






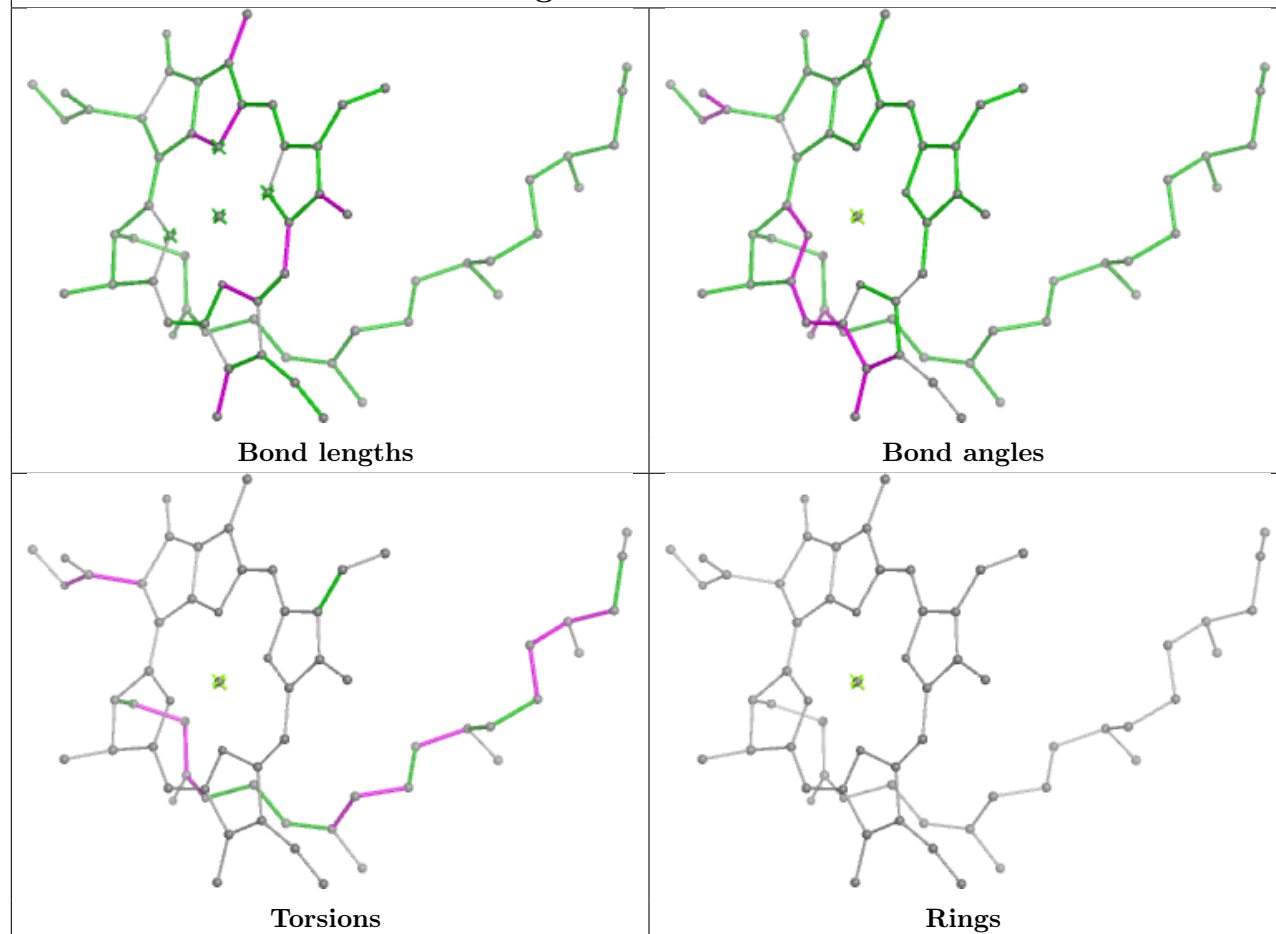


## Ligand CLA a 840

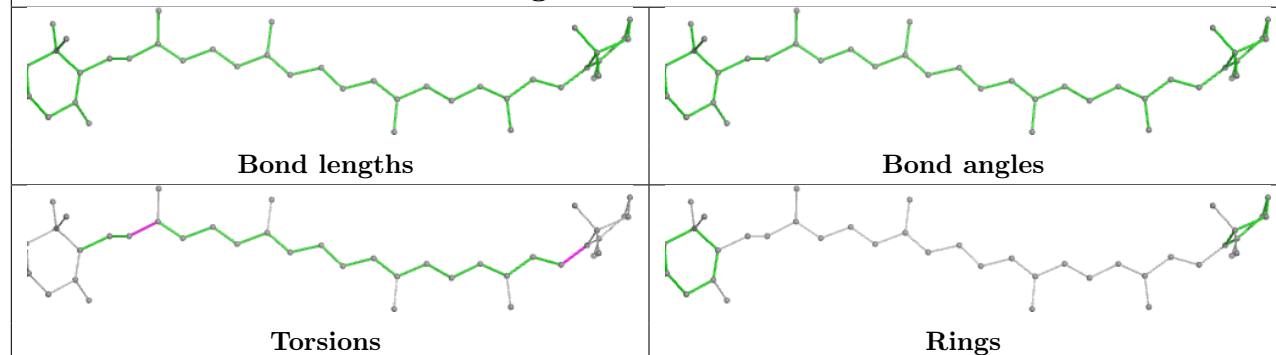




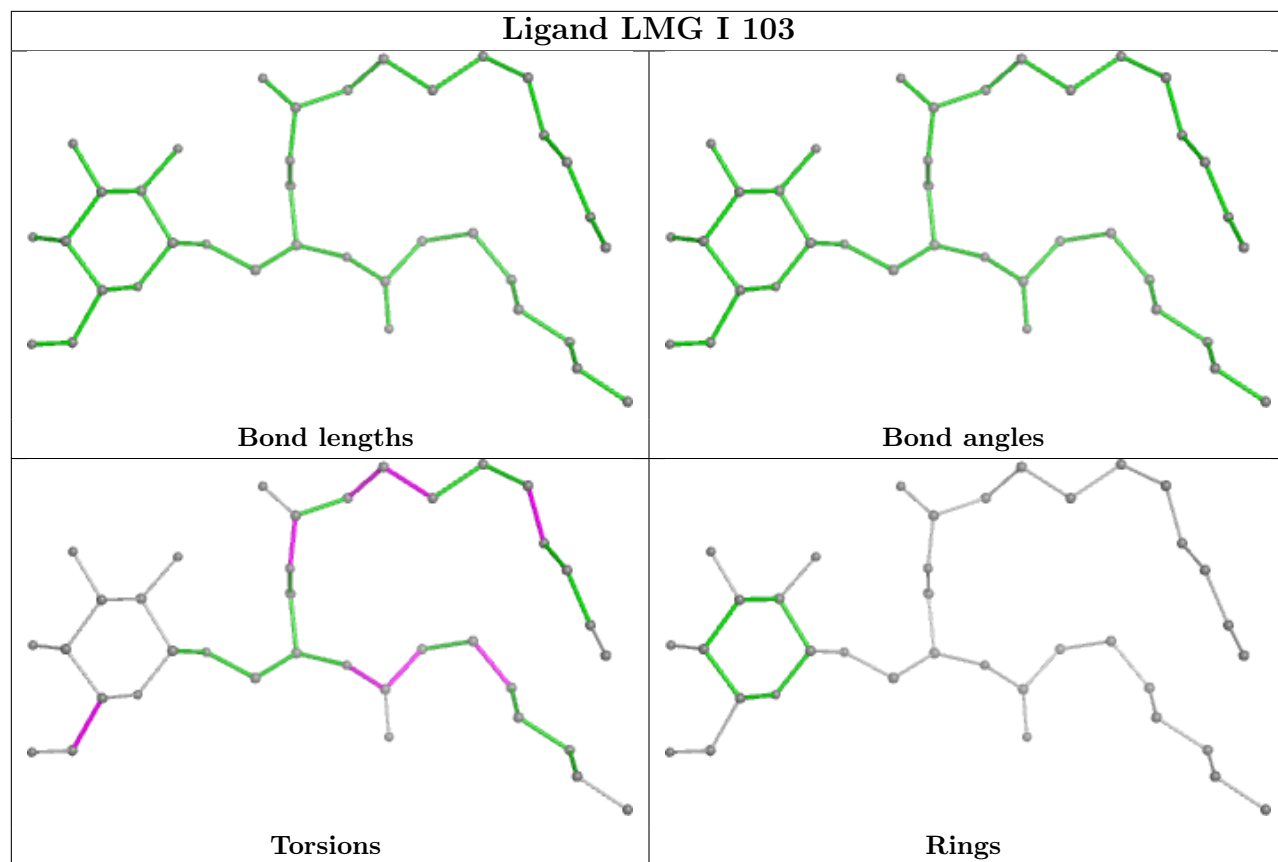
## Ligand CLA b 827



## Ligand BCR A 849

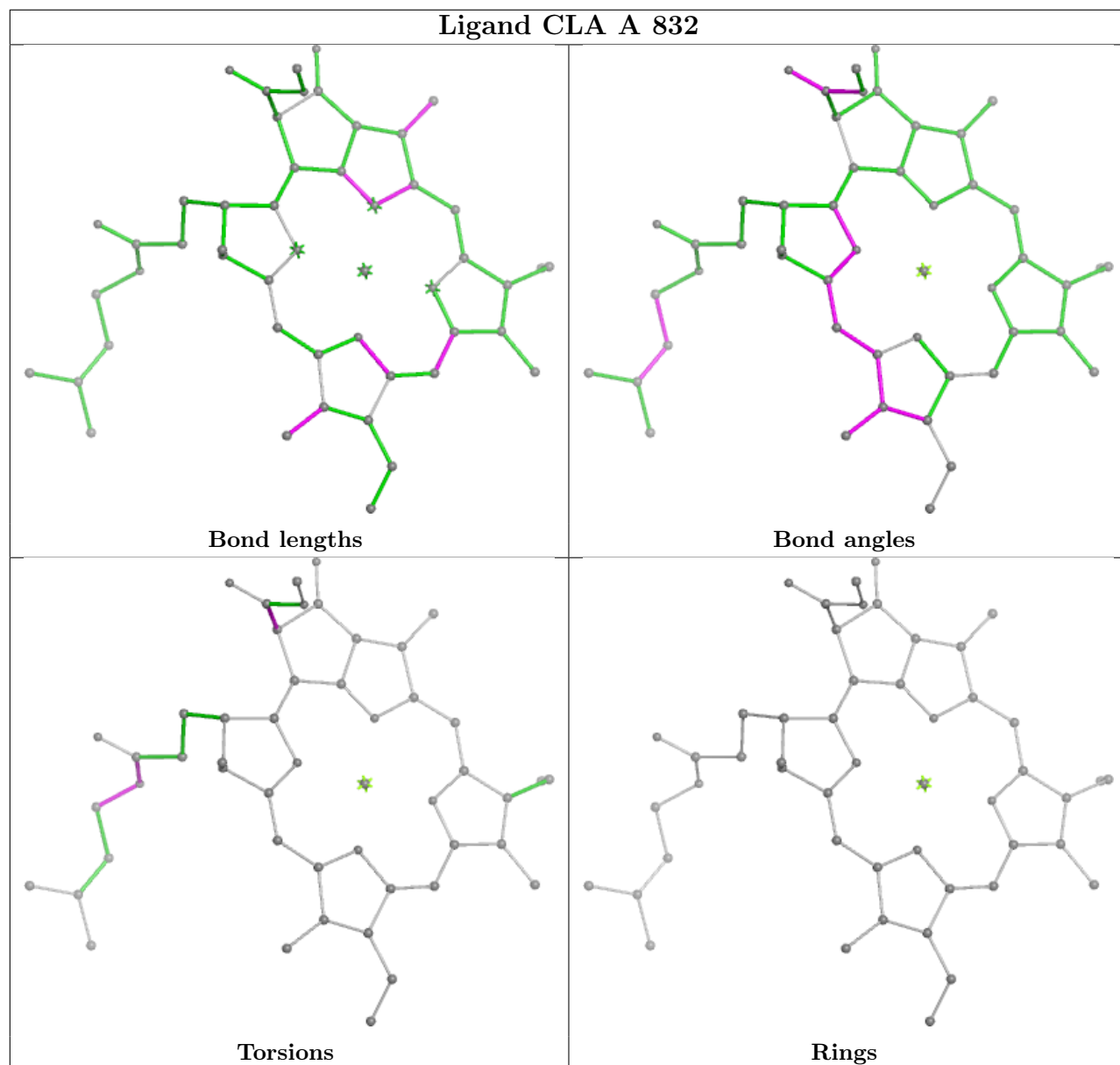






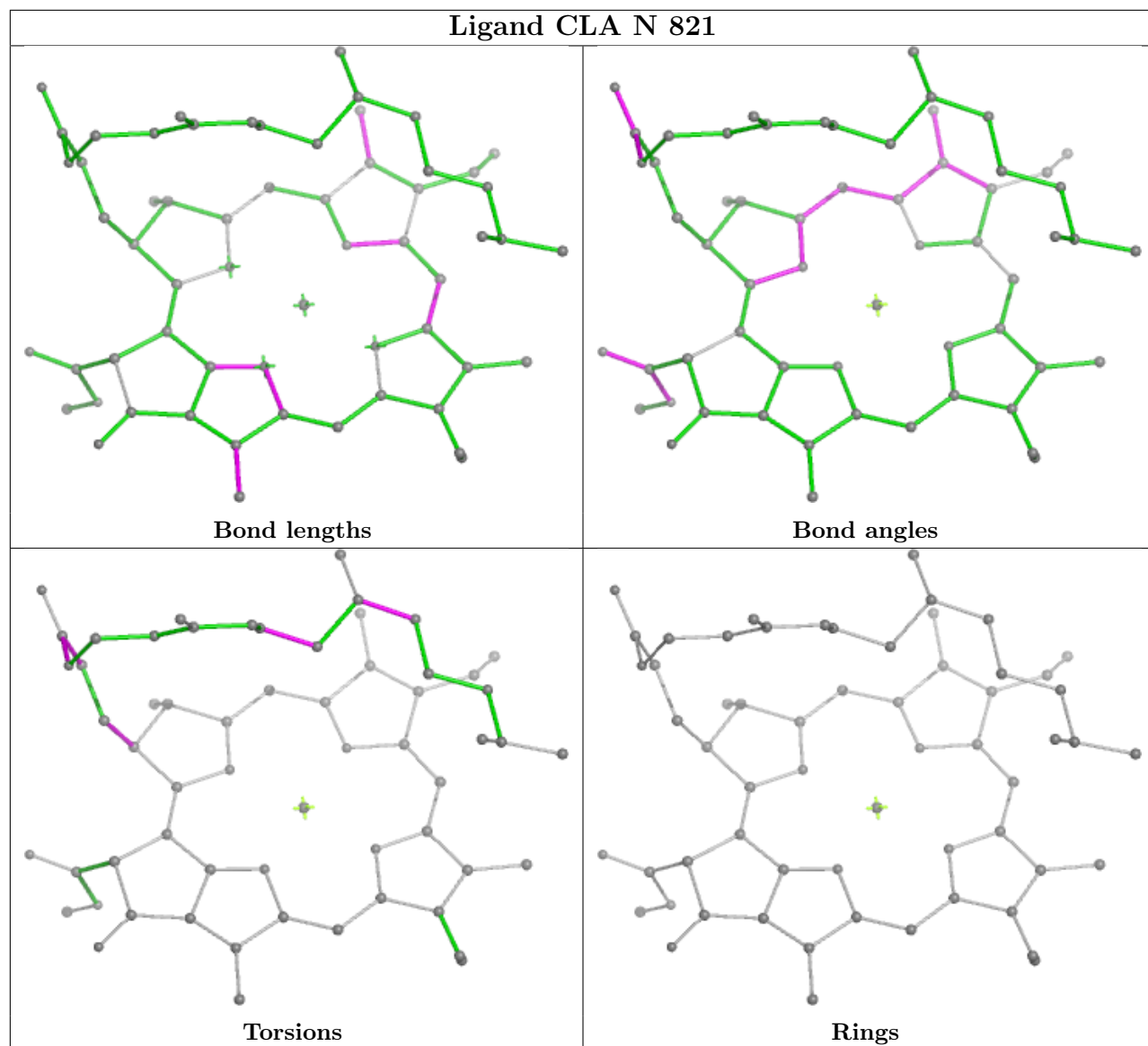


## Ligand CLA A 832

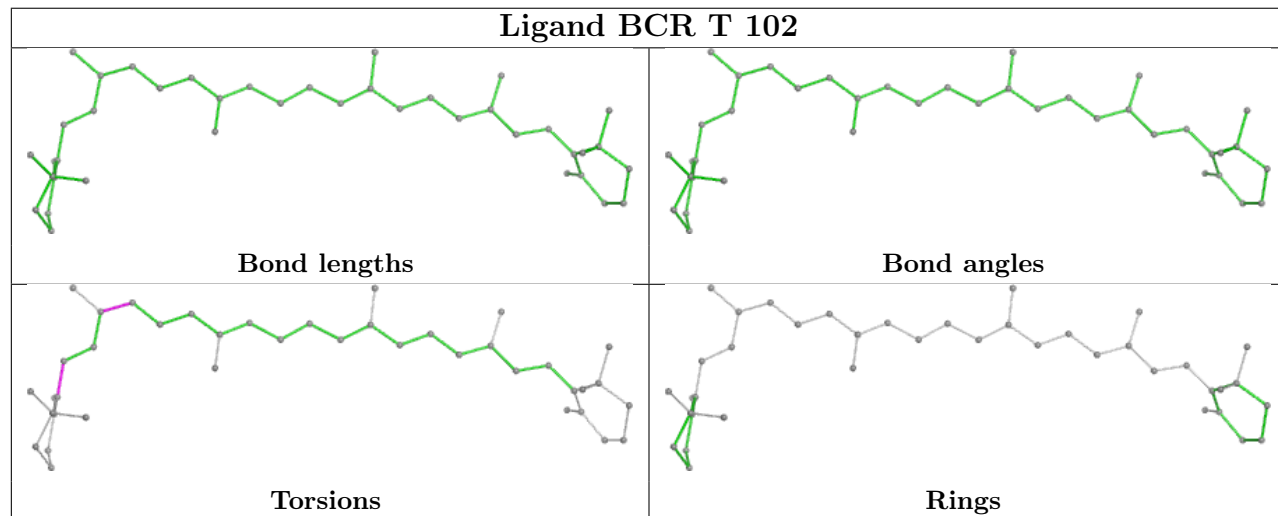




## Ligand CLA N 821

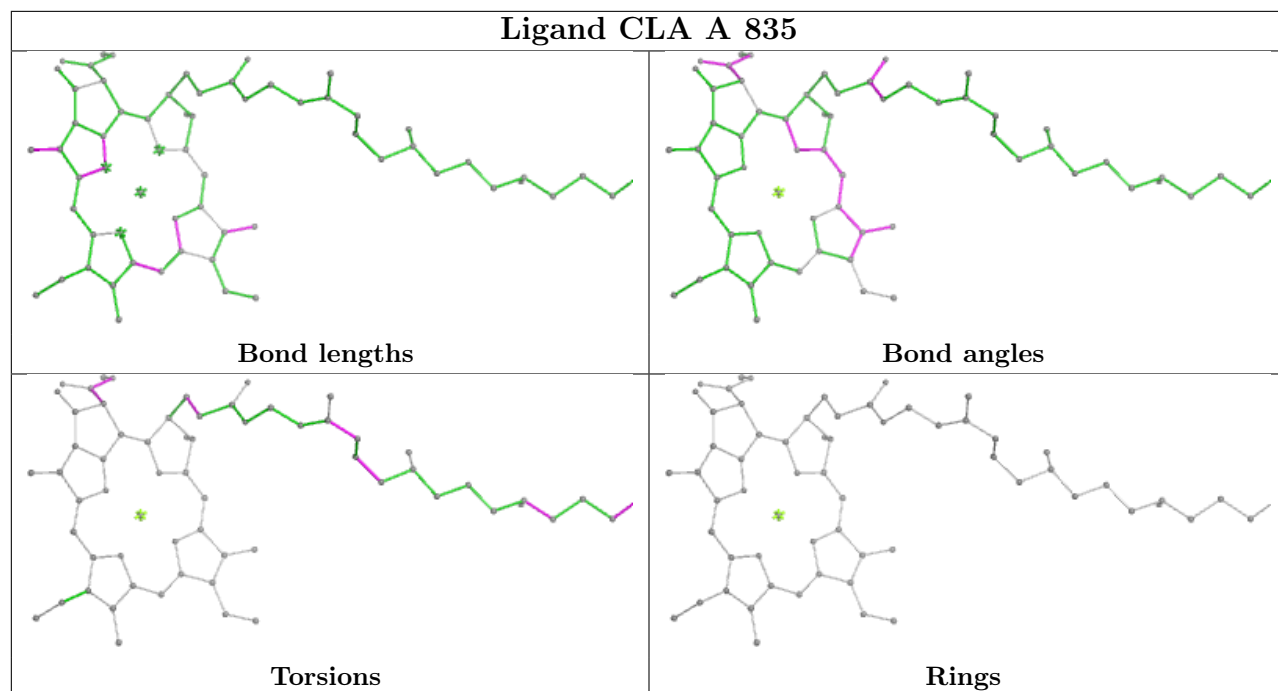


## Ligand BCR T 102

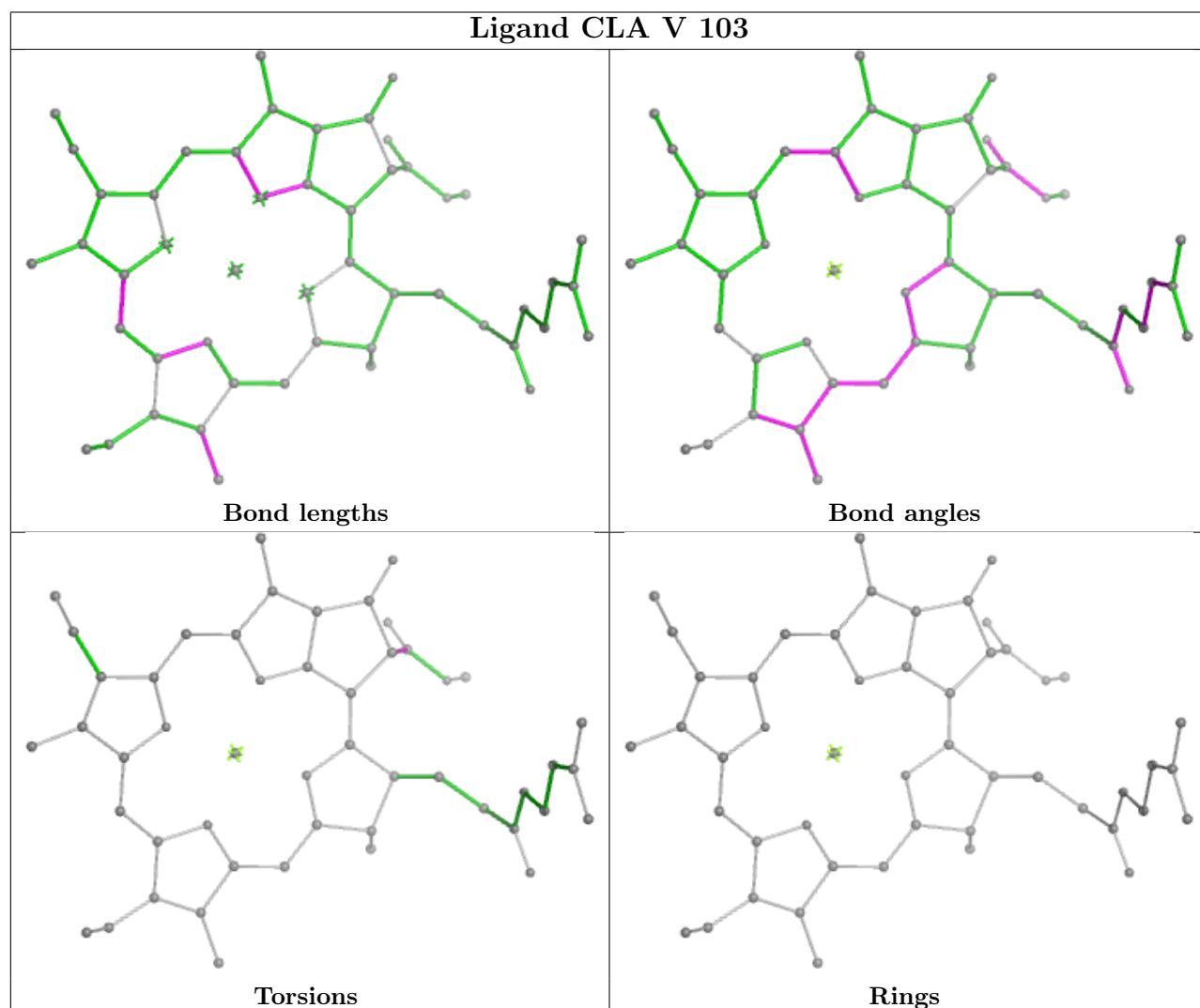




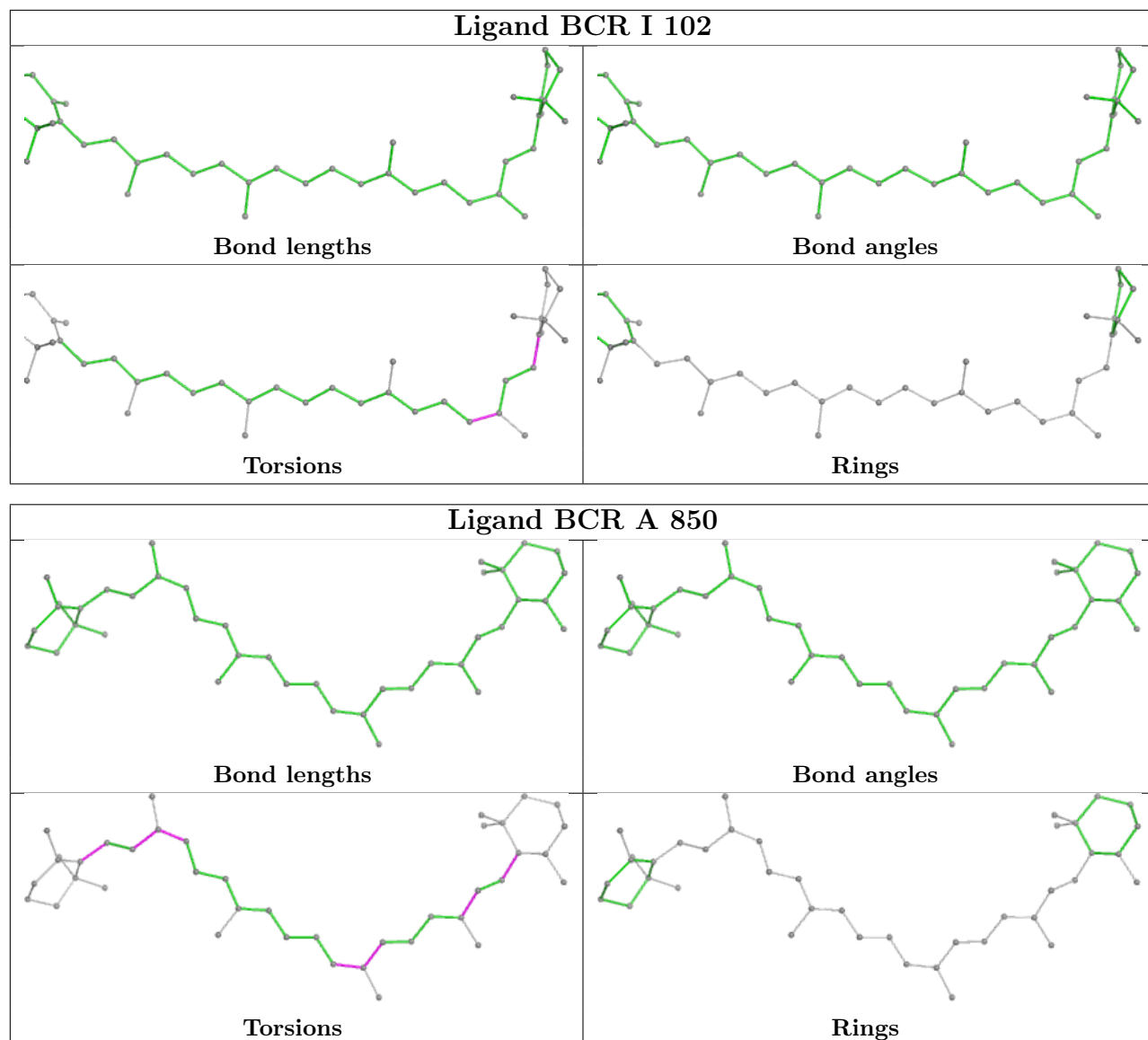
## Ligand CLA A 835



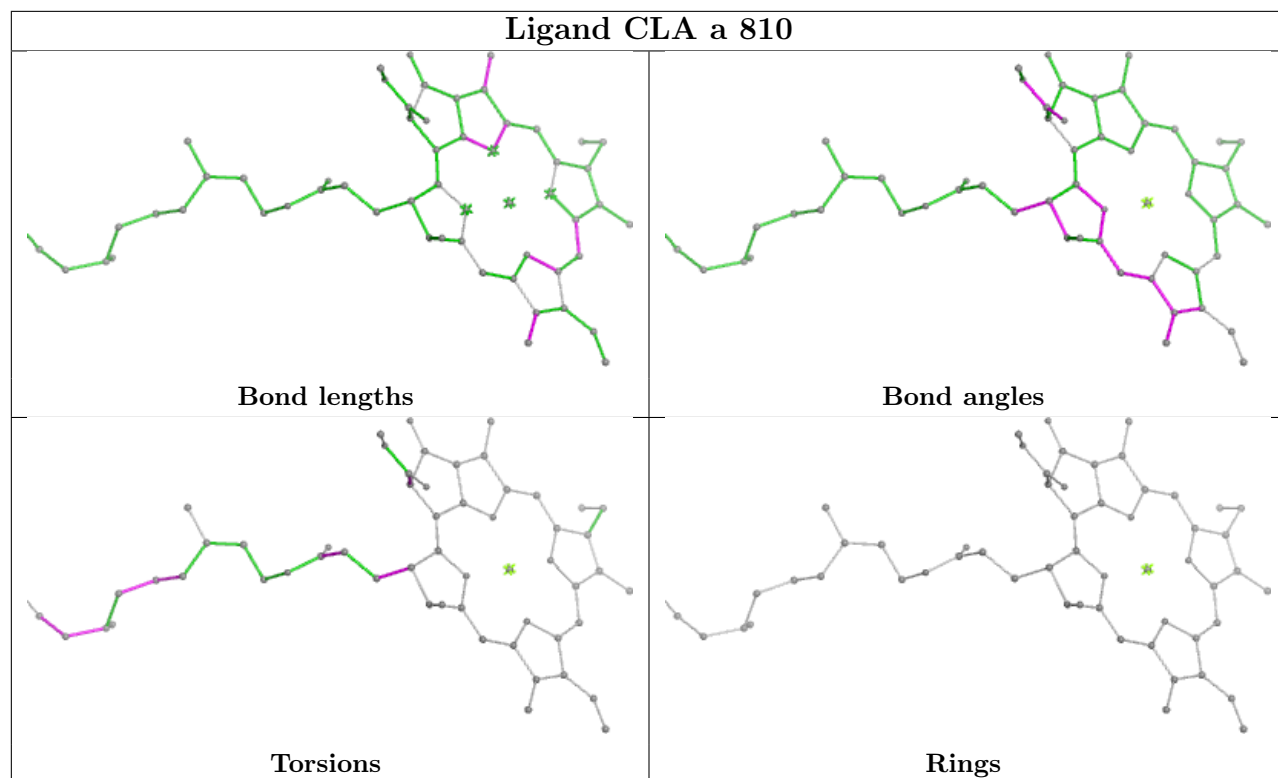
## Ligand CLA V 103





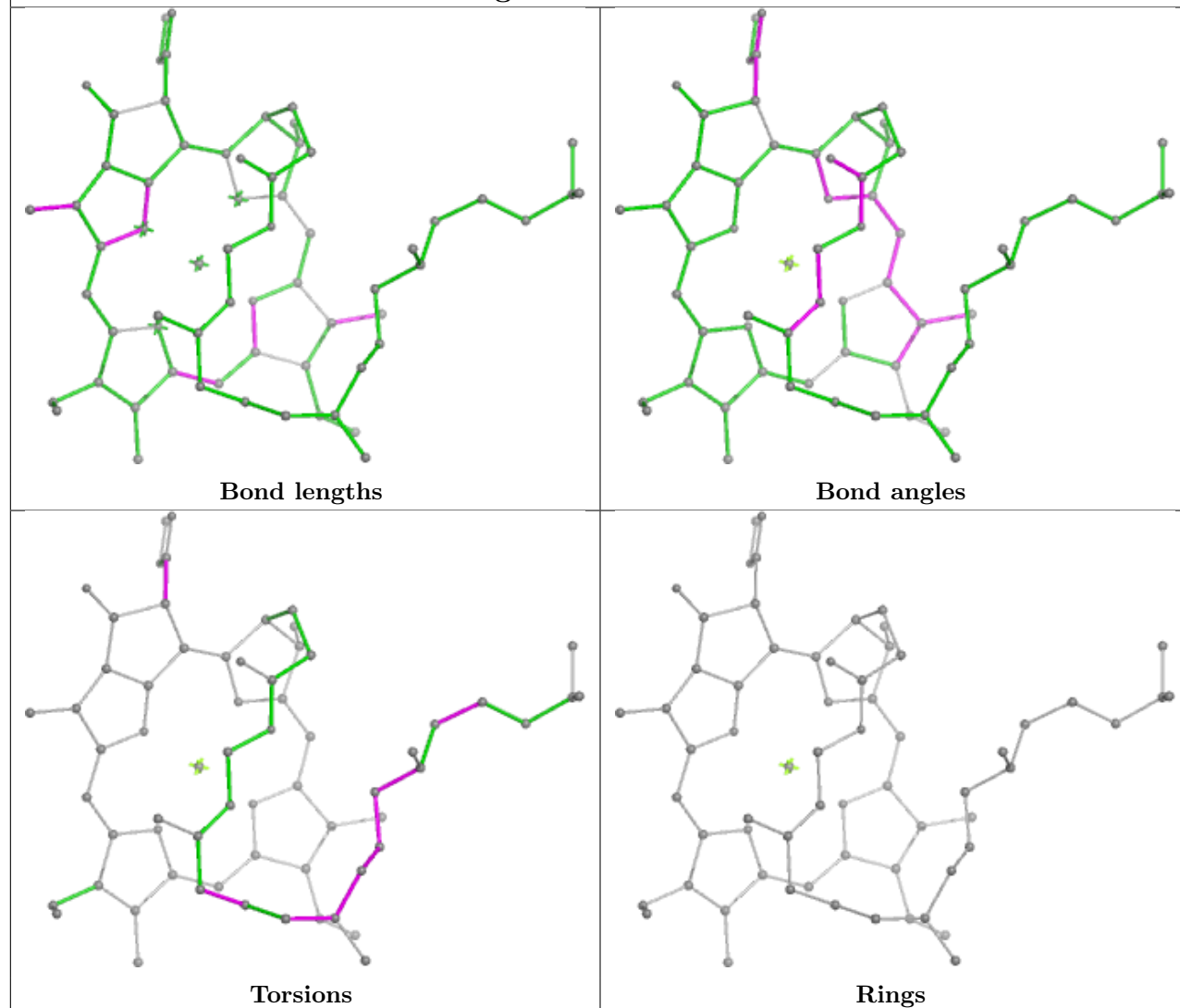




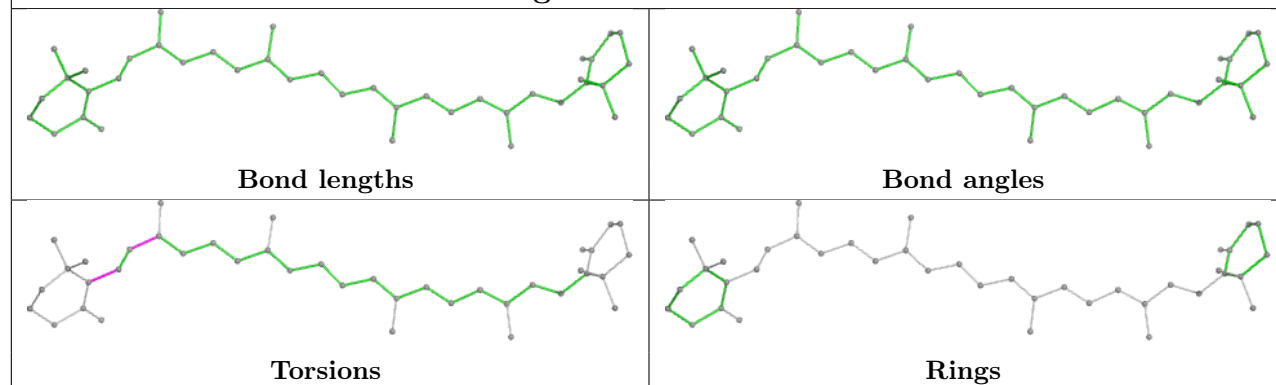




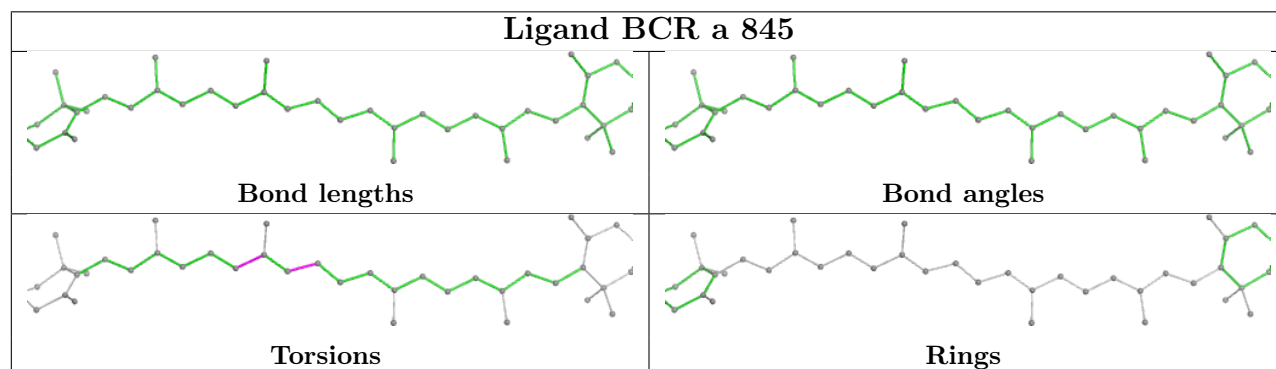
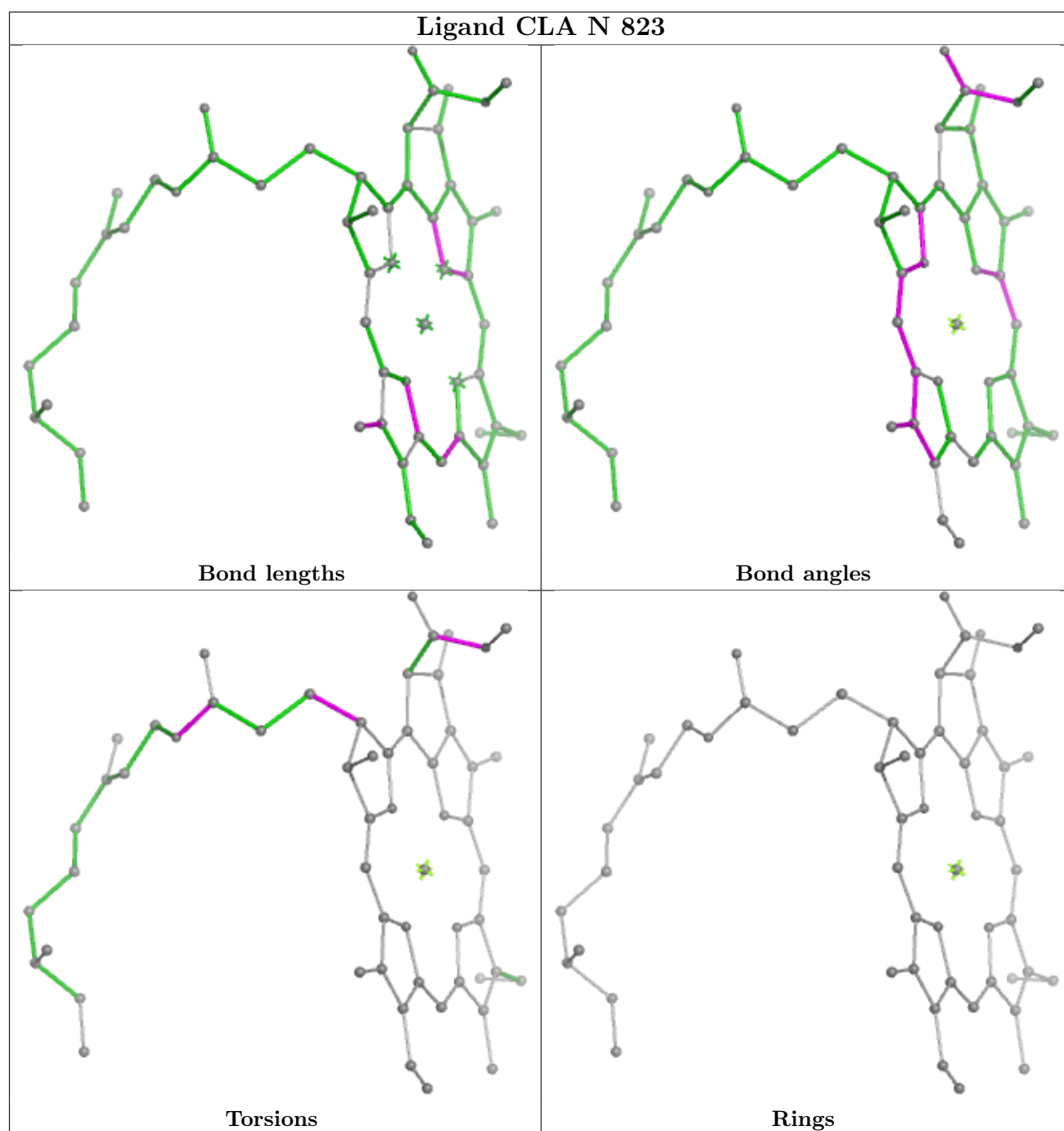
## Ligand CLA b 808



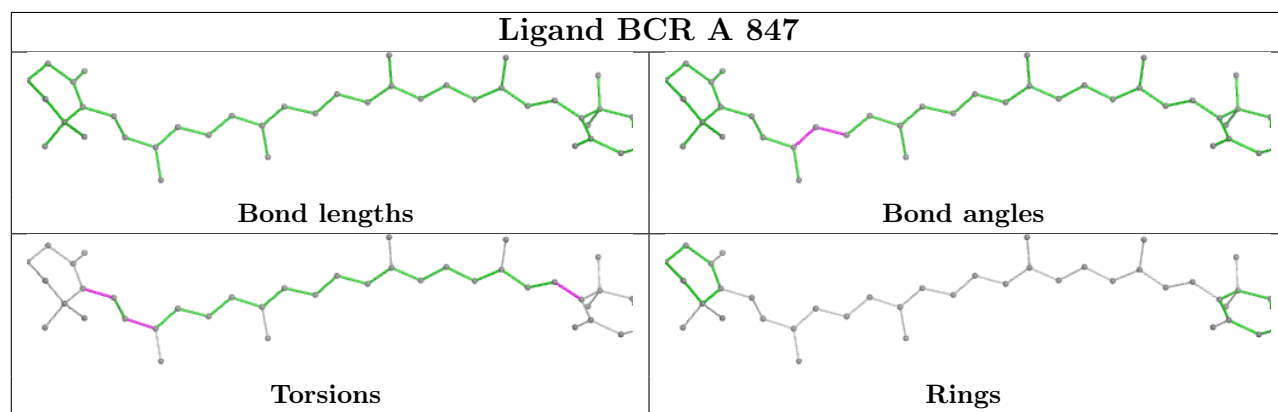
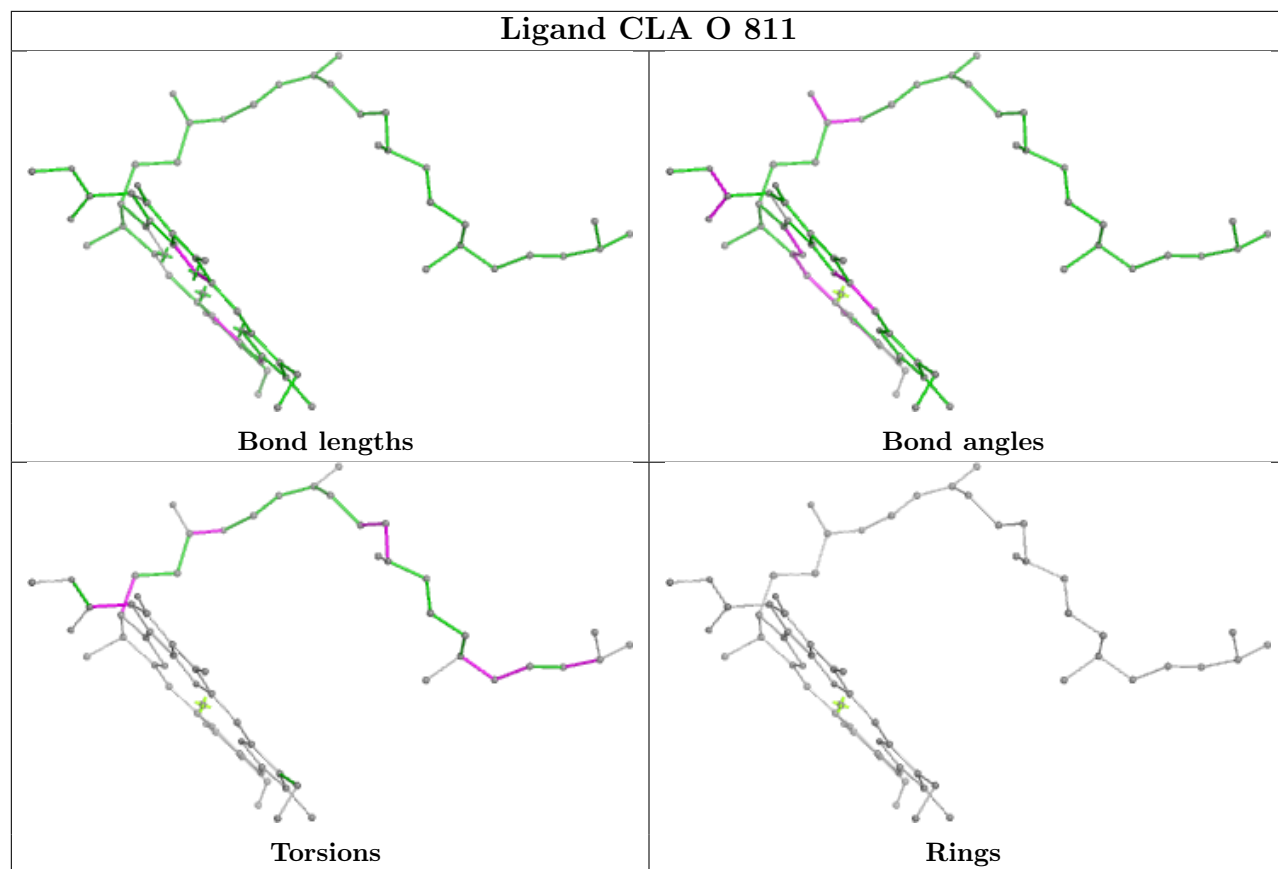
## Ligand BCR b 848



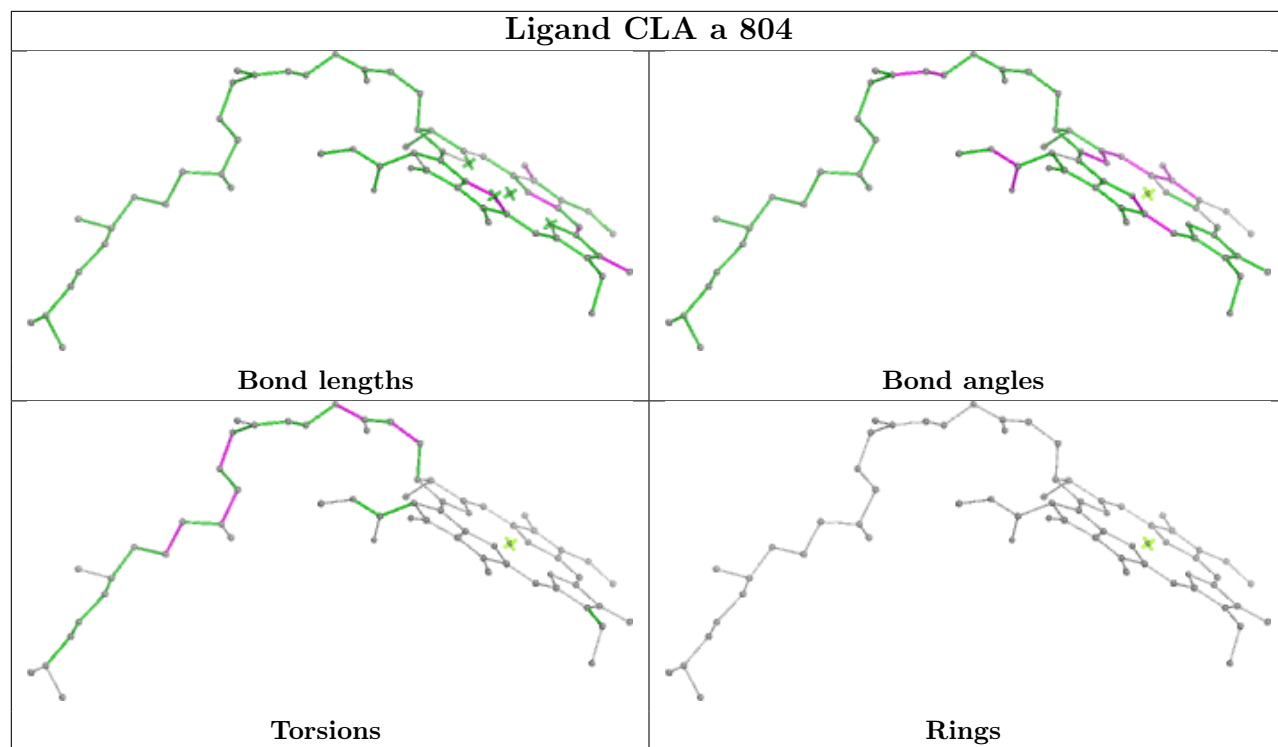






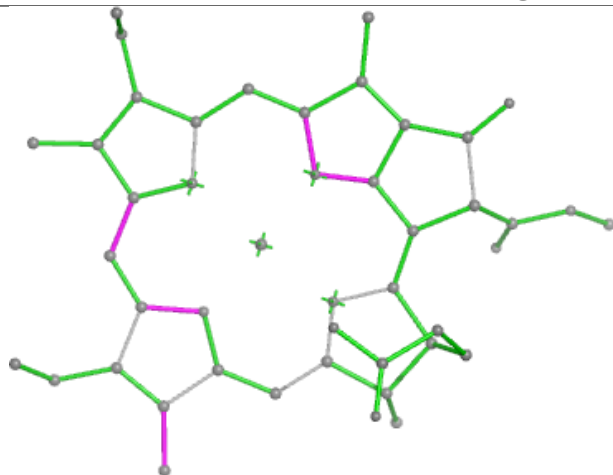




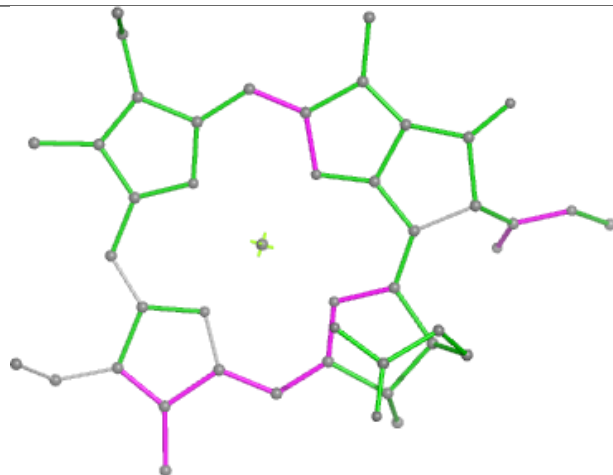




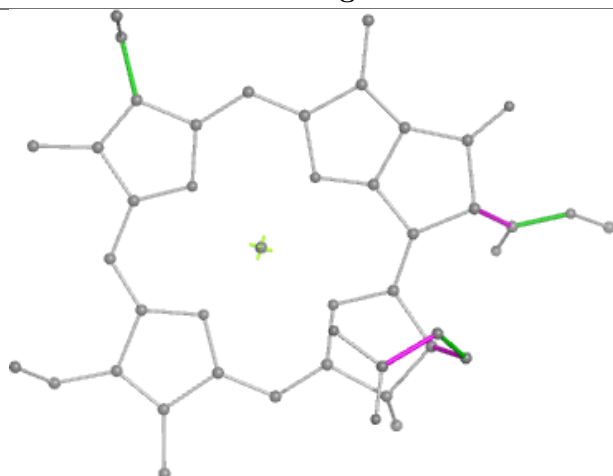
## Ligand CLA B 810



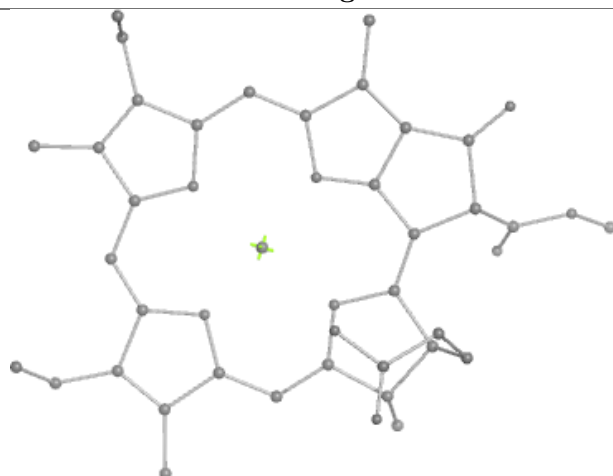
Bond lengths



Bond angles

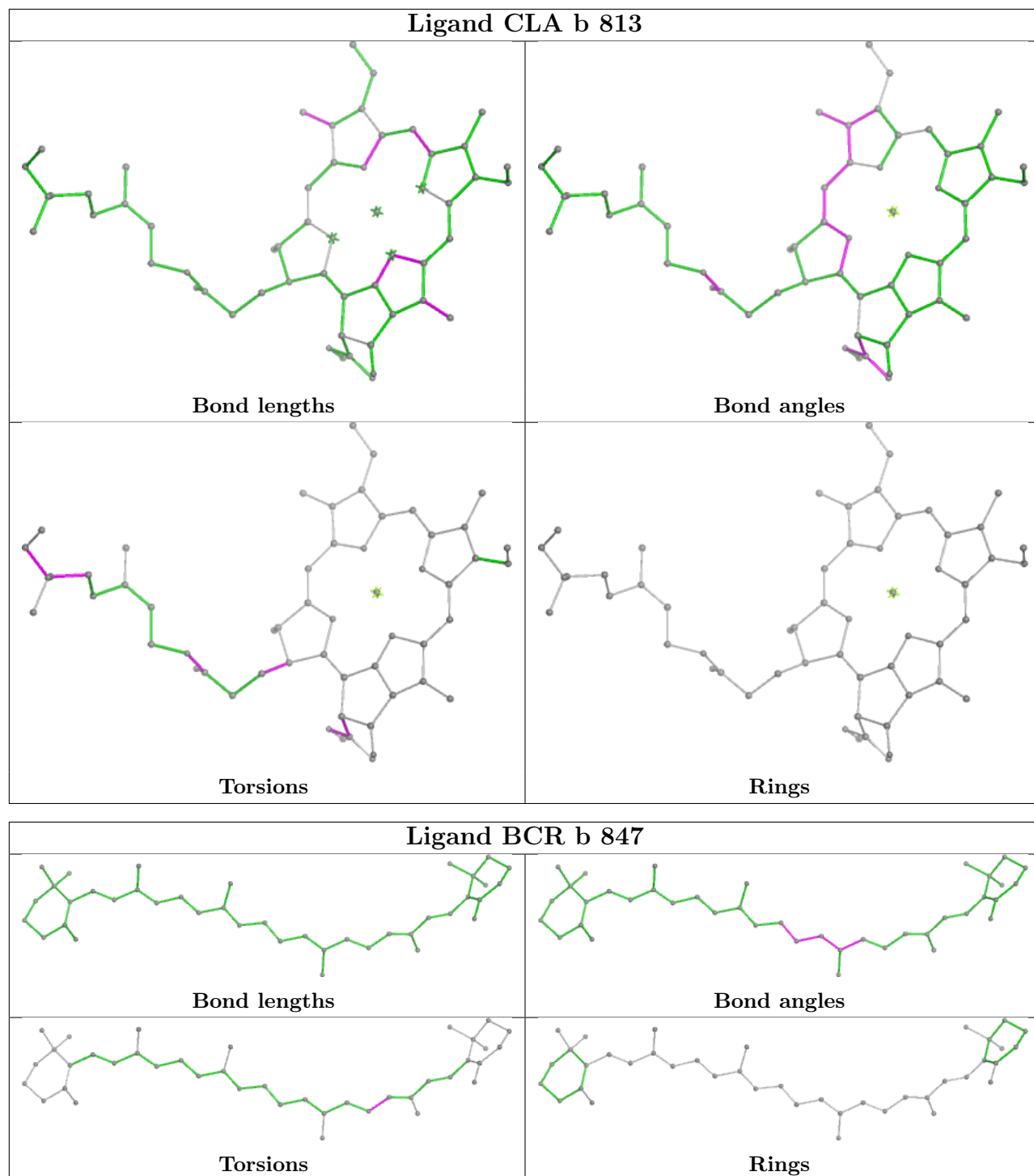


Torsions



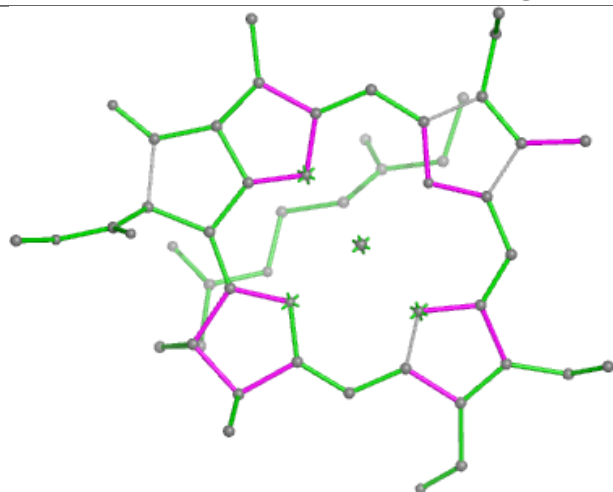
Rings



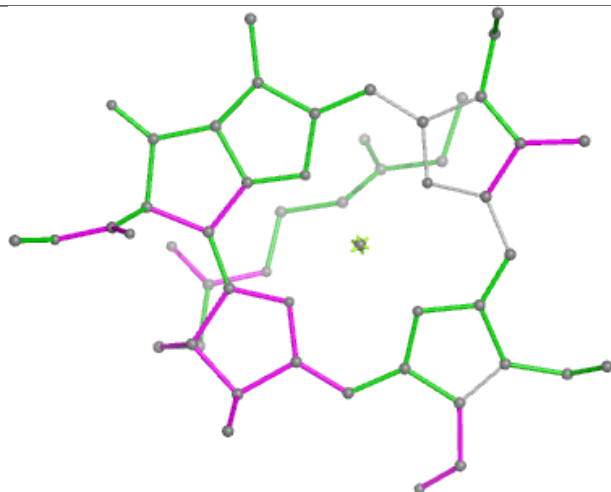




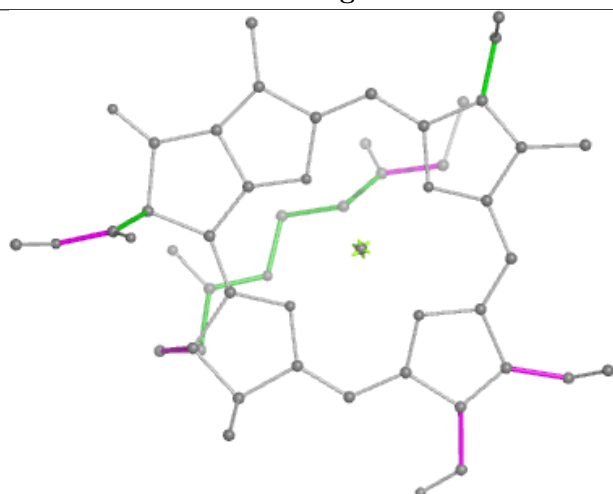
## Ligand F6C N 824



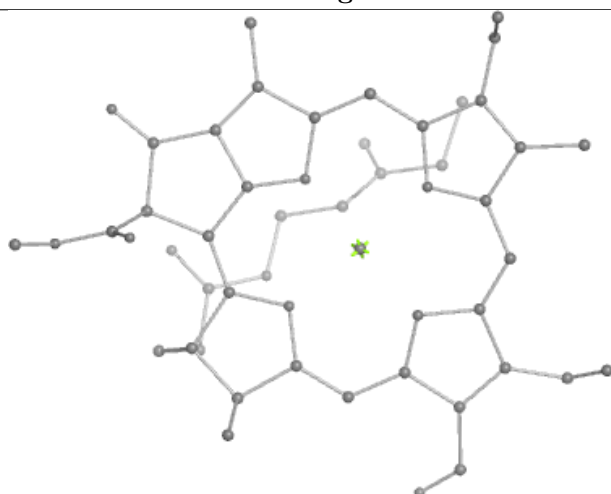
Bond lengths



Bond angles

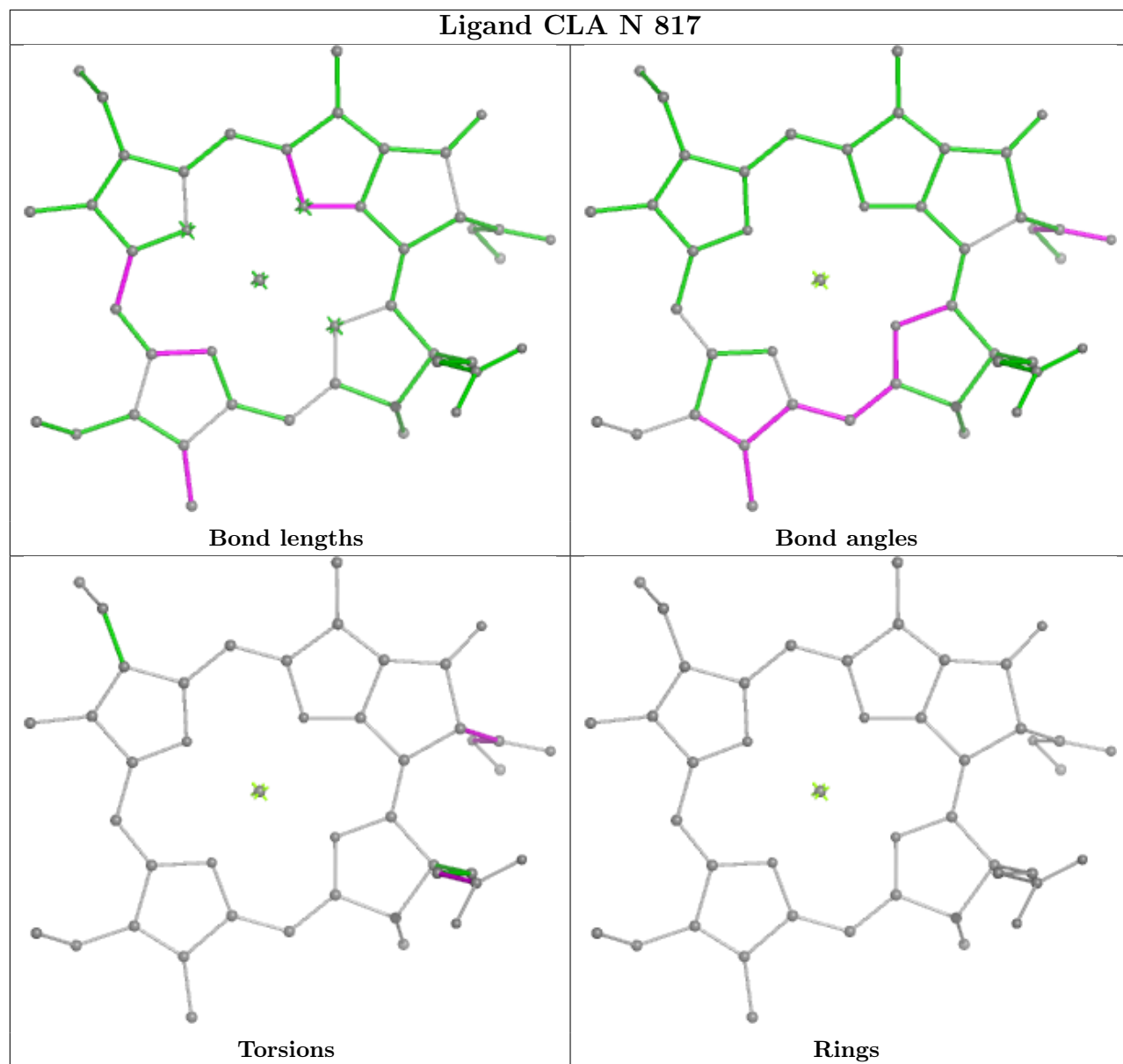


Torsions

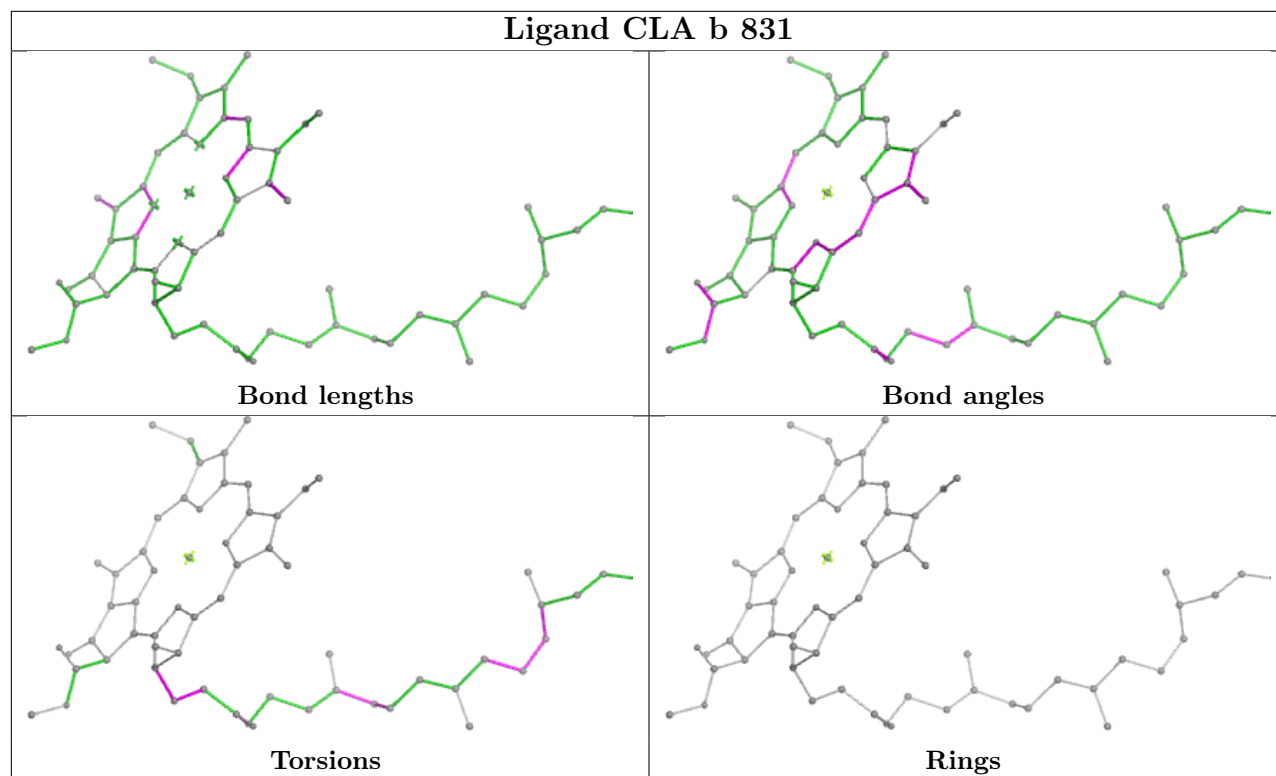
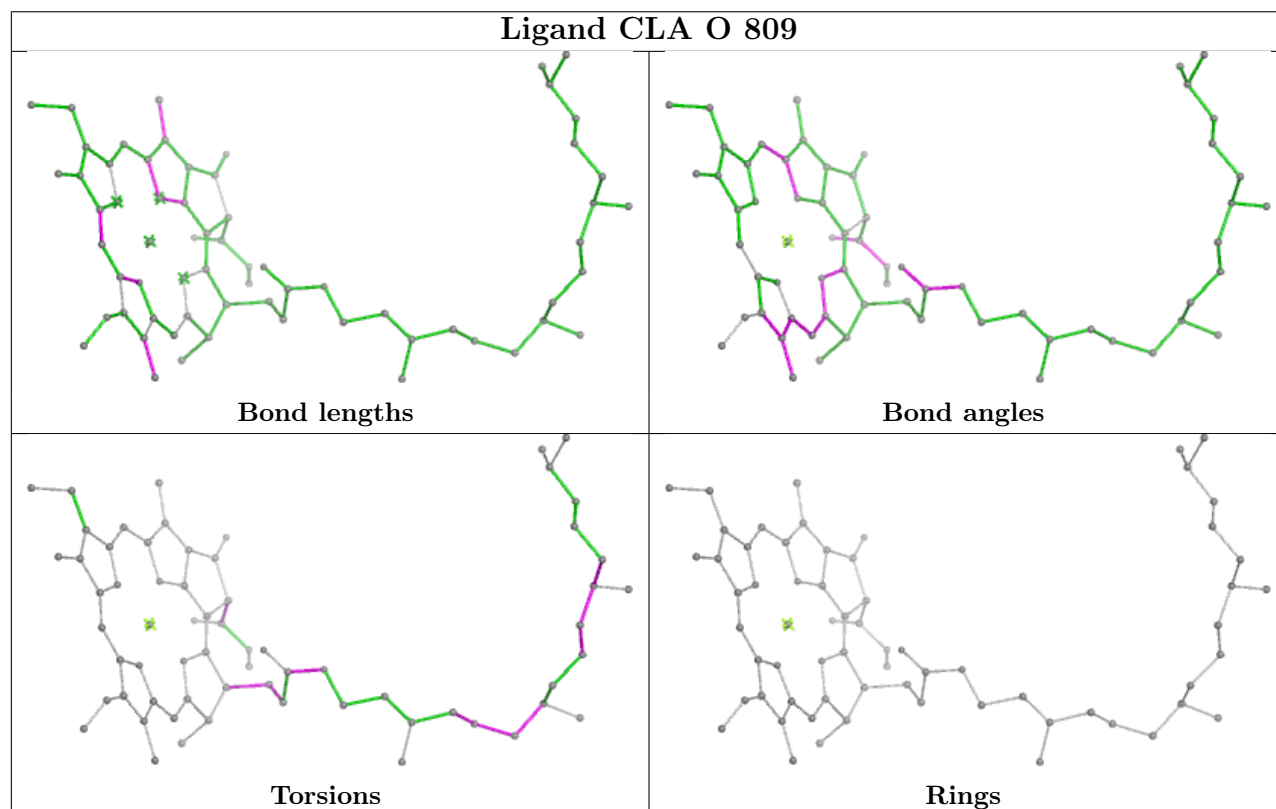


Rings

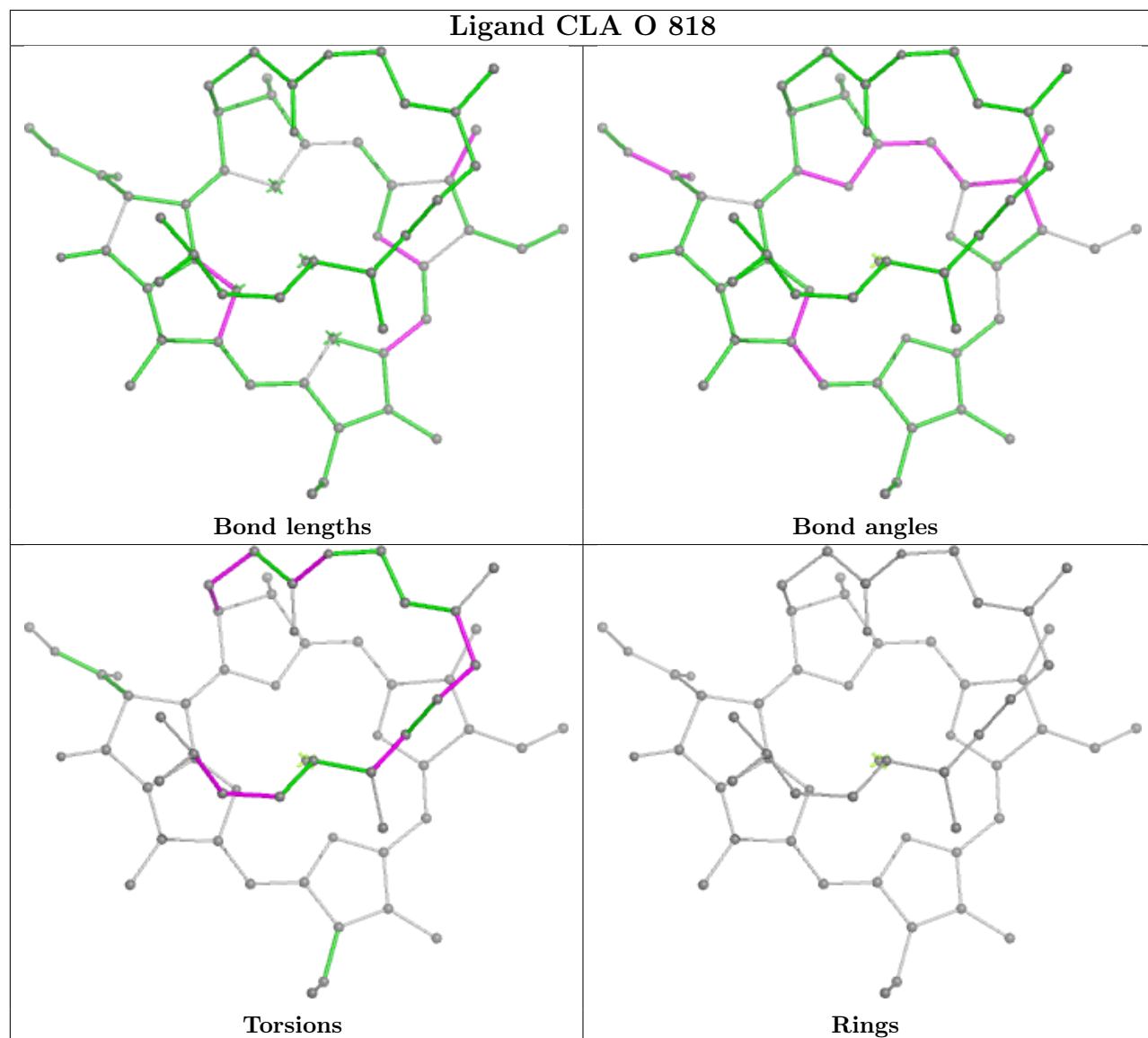




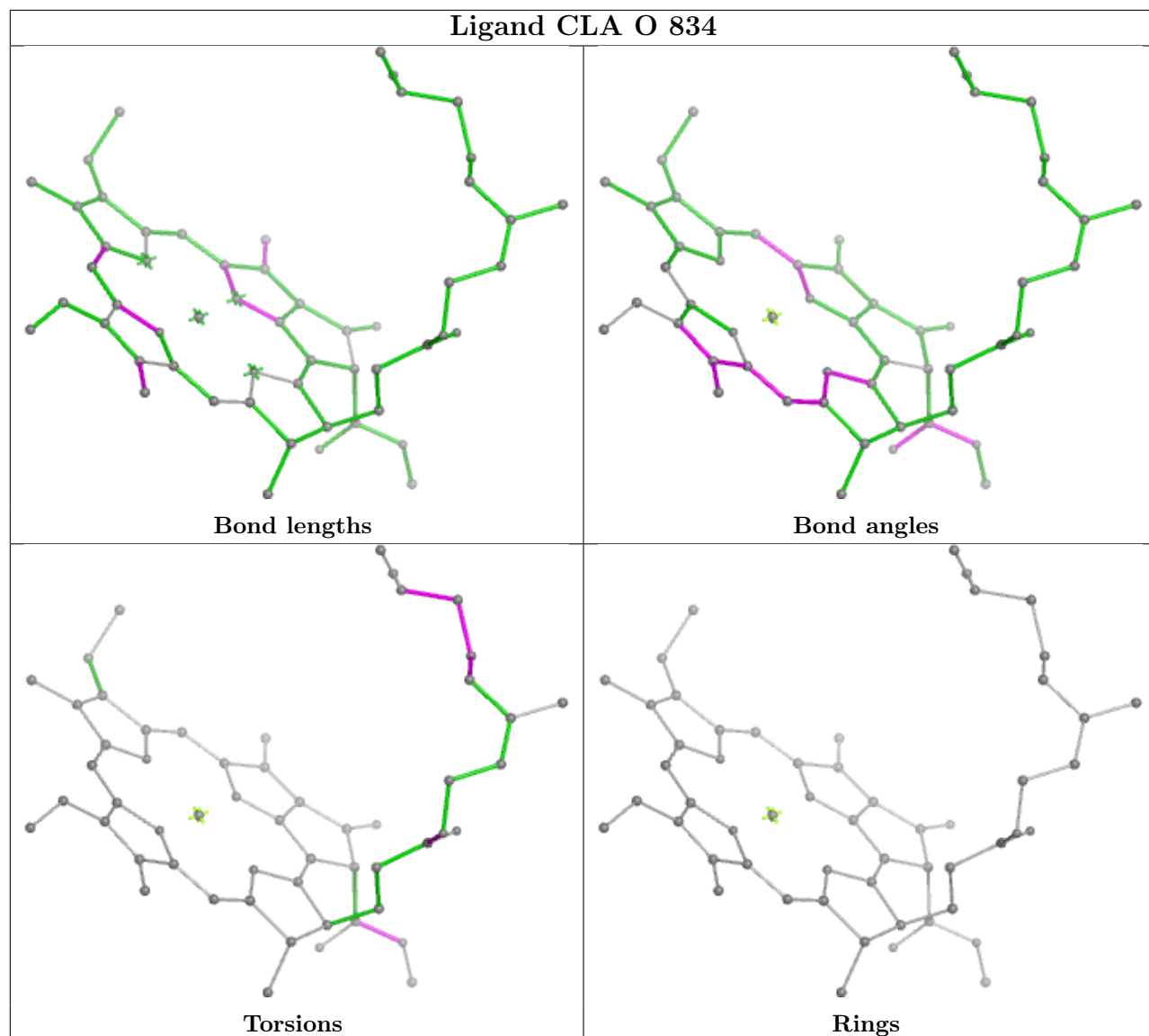


**Ligand CLA b 831****Ligand CLA O 809**

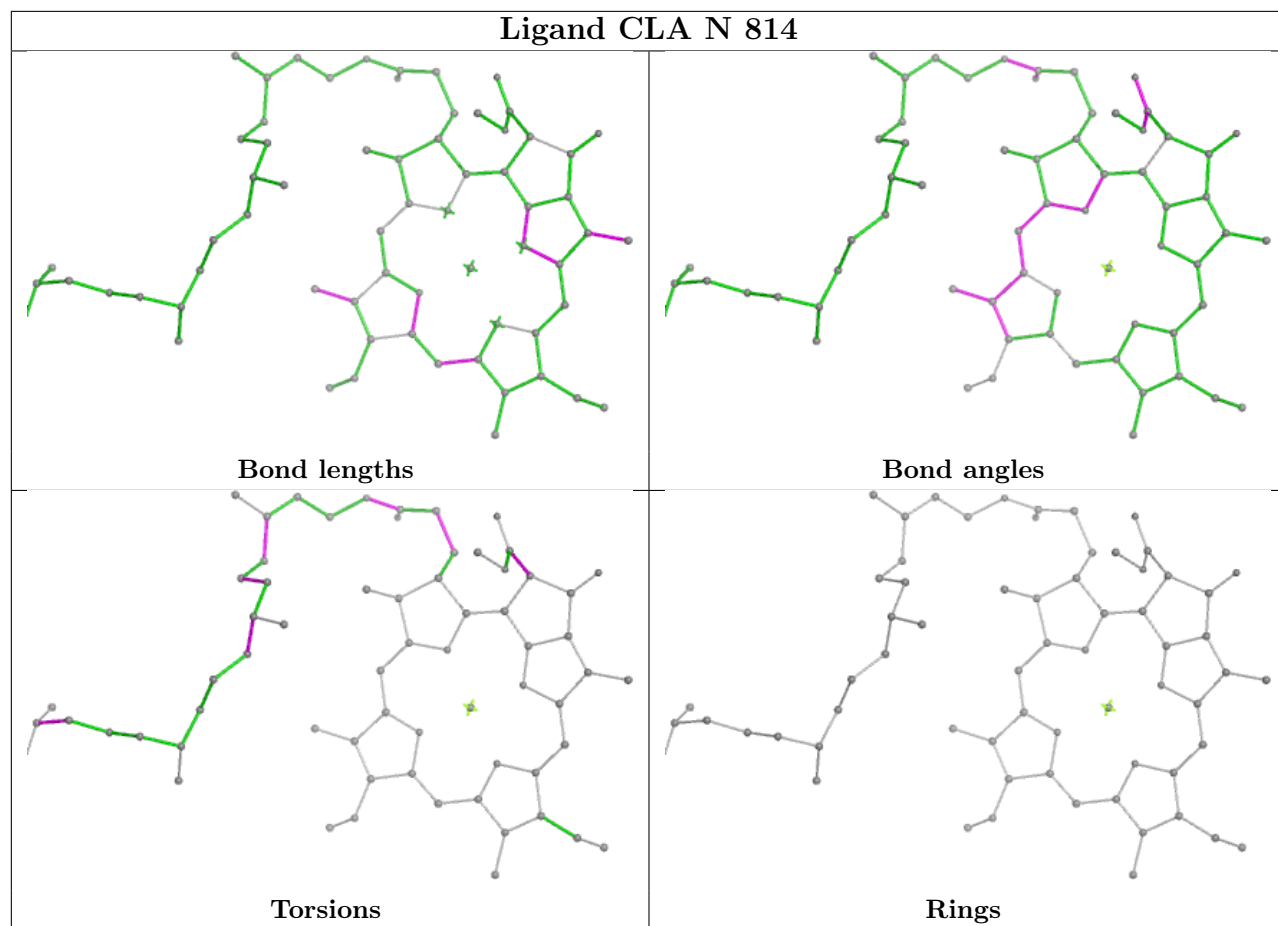






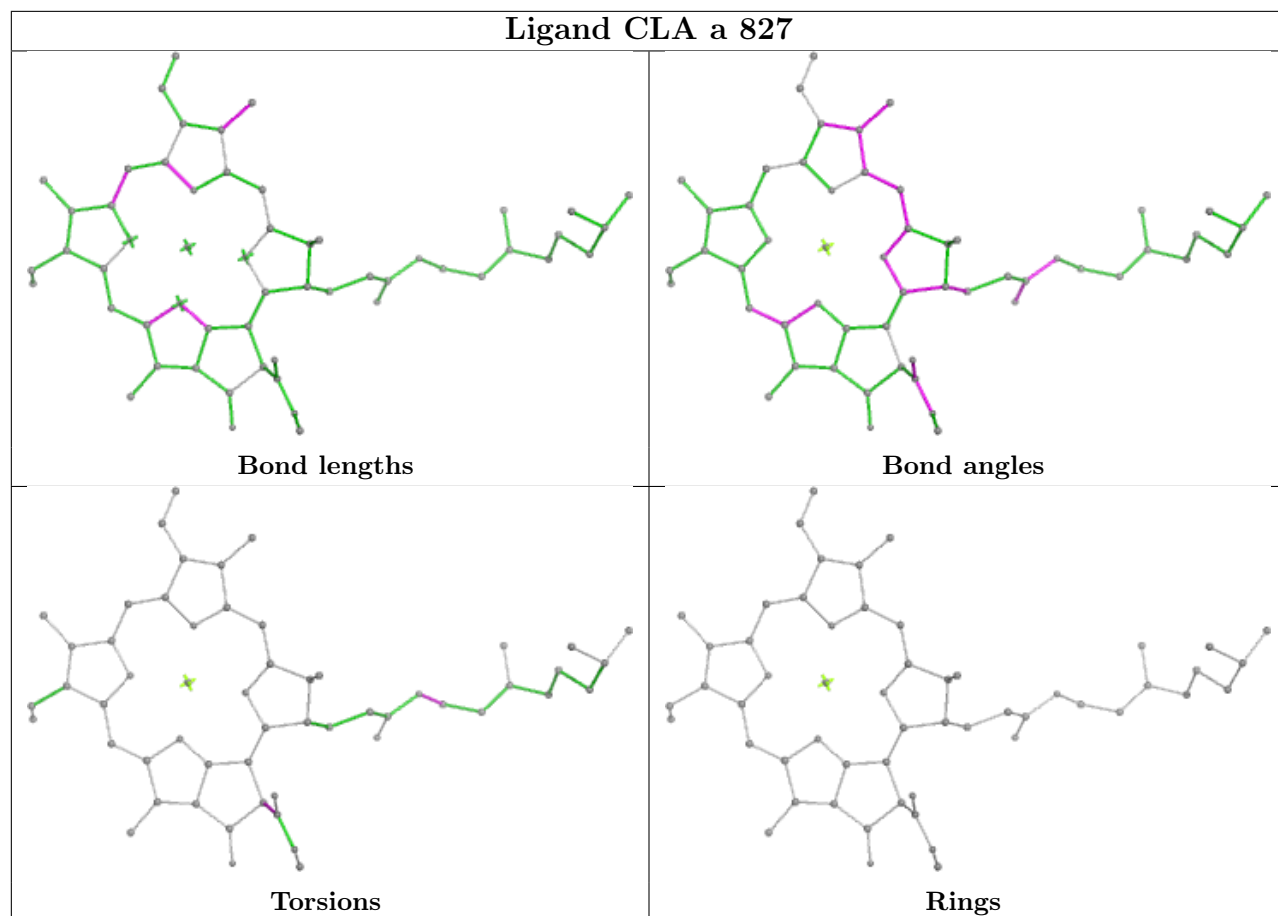




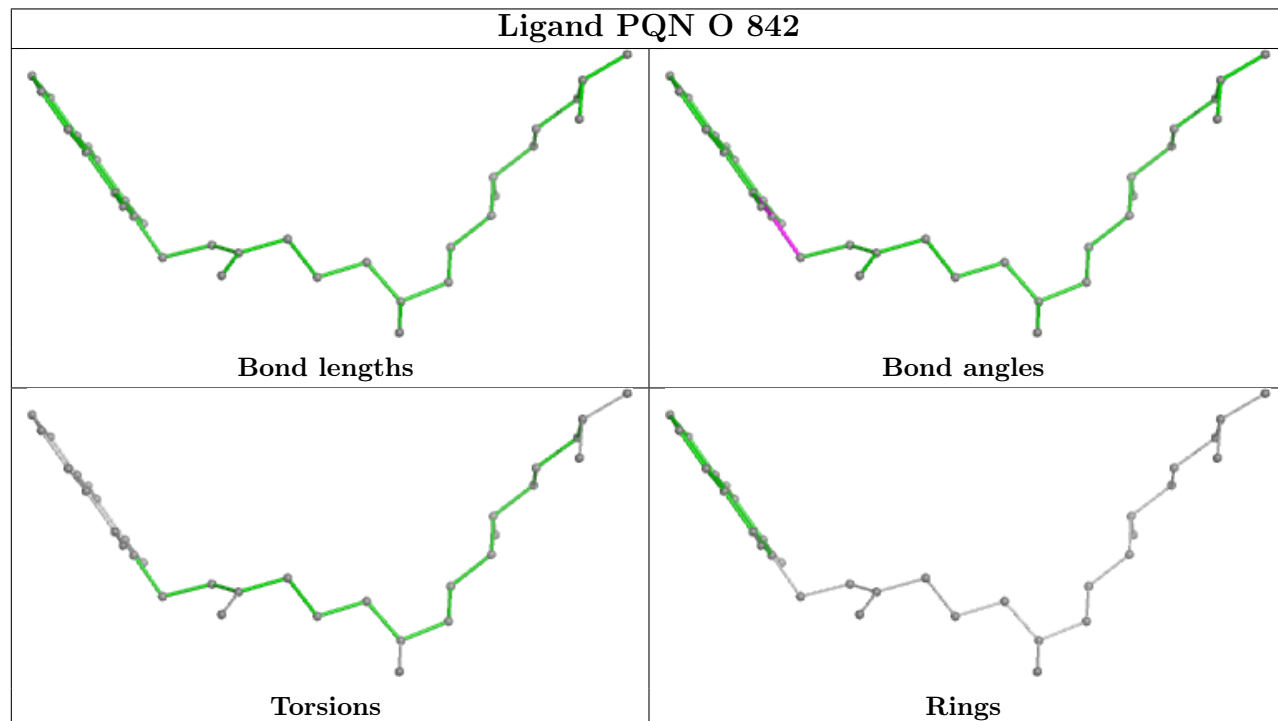




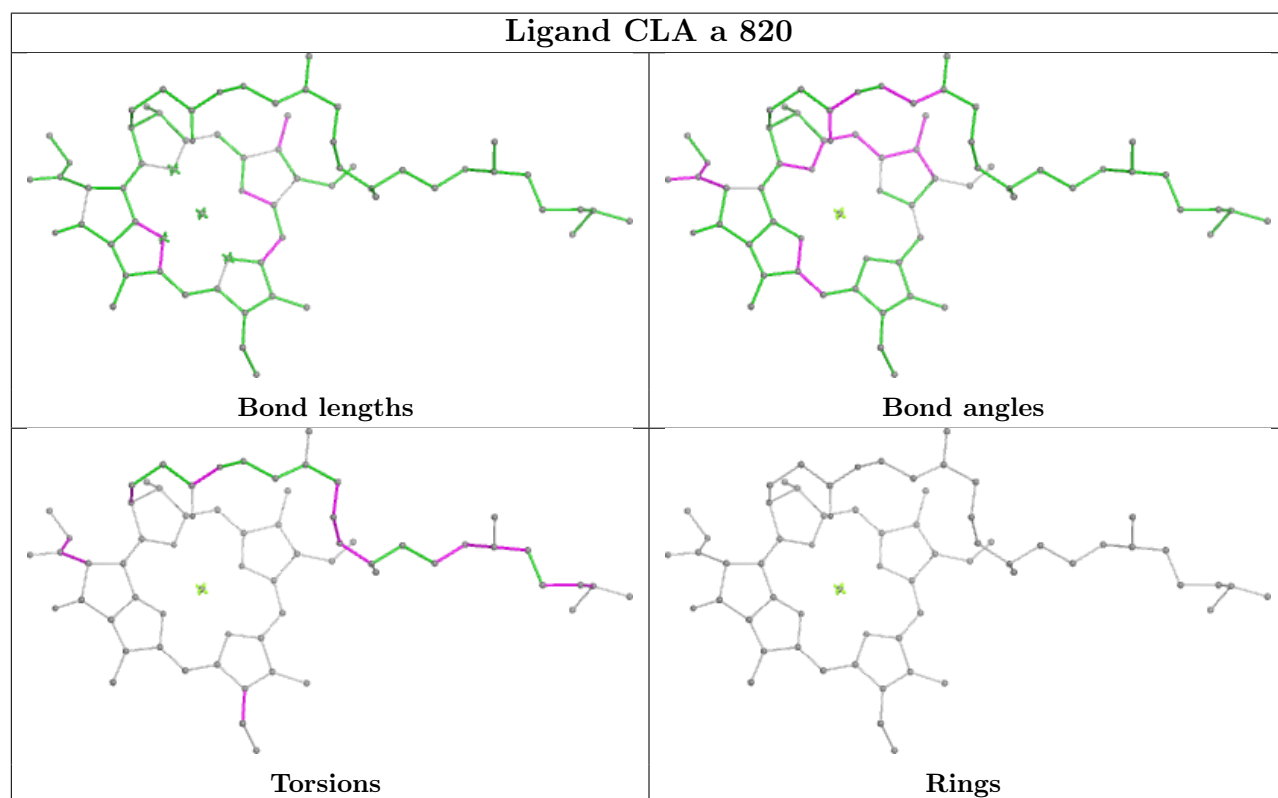
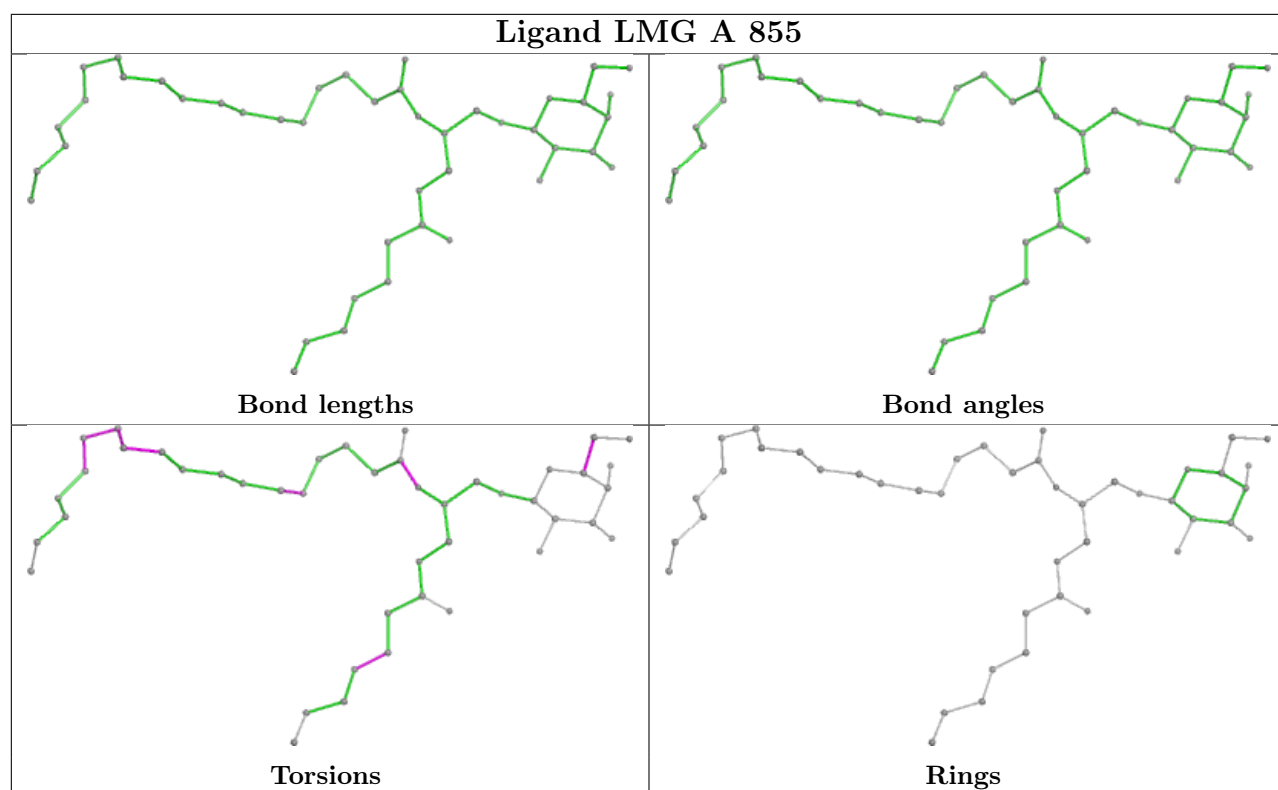
## Ligand CLA a 827



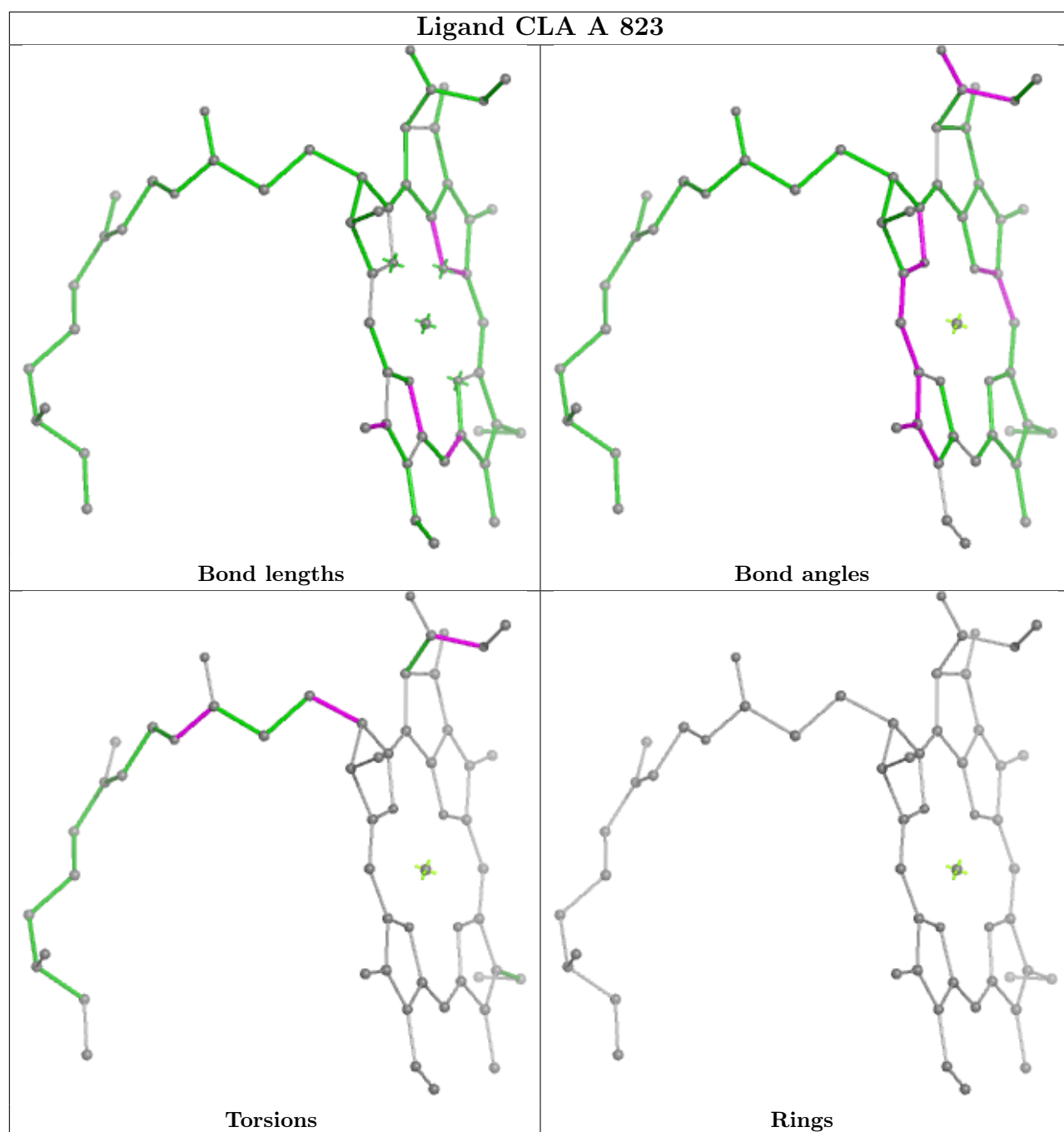
## Ligand PQN O 842



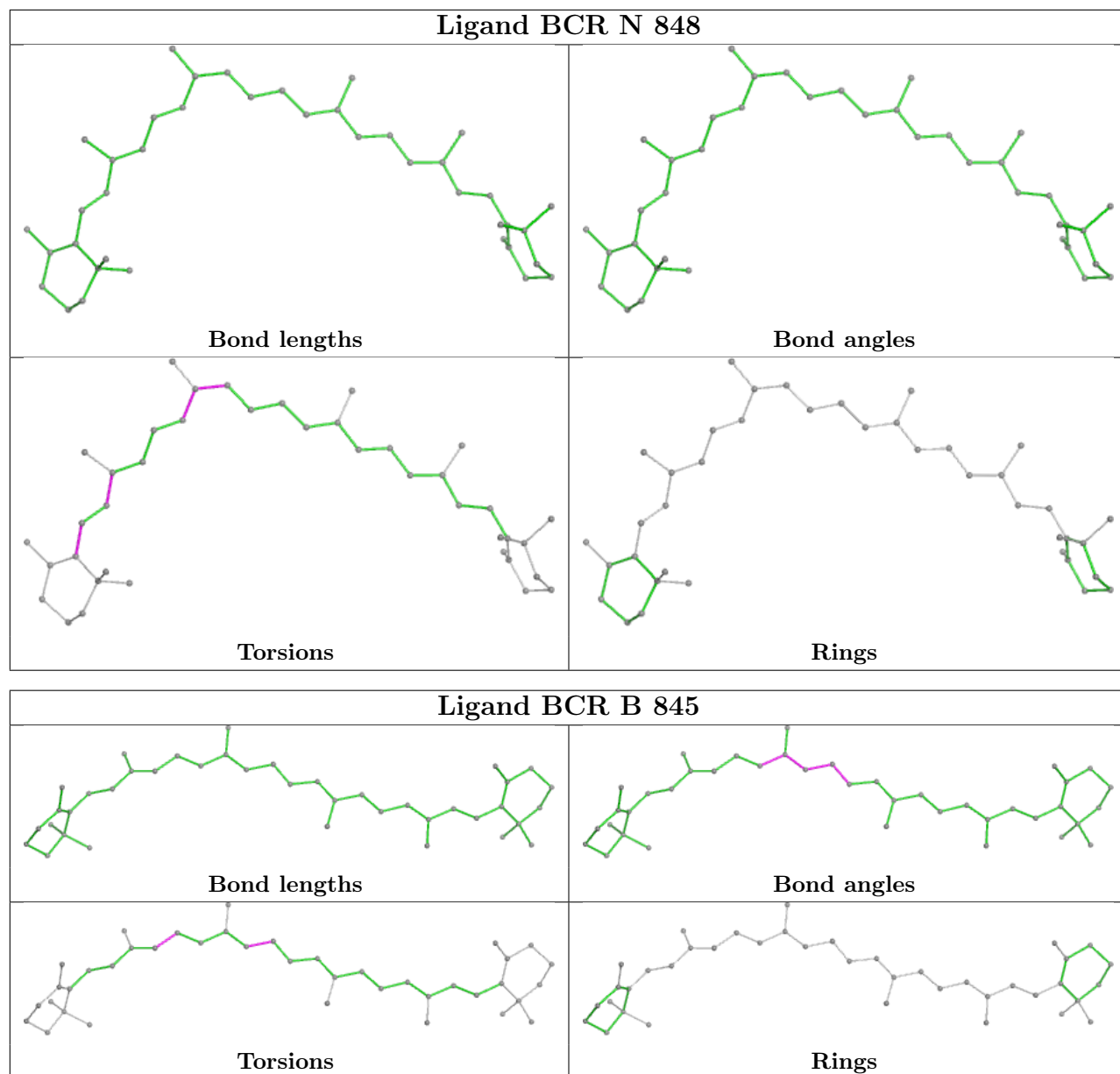




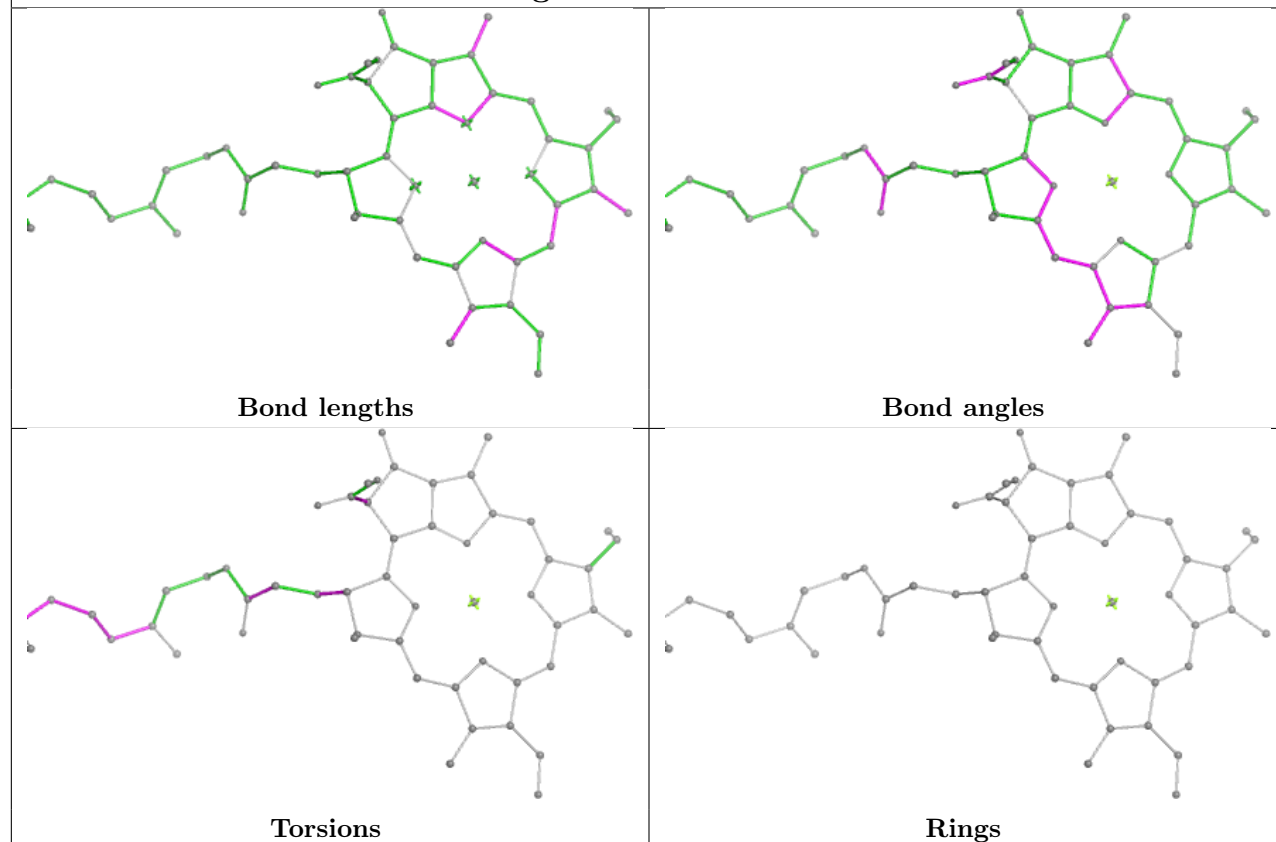
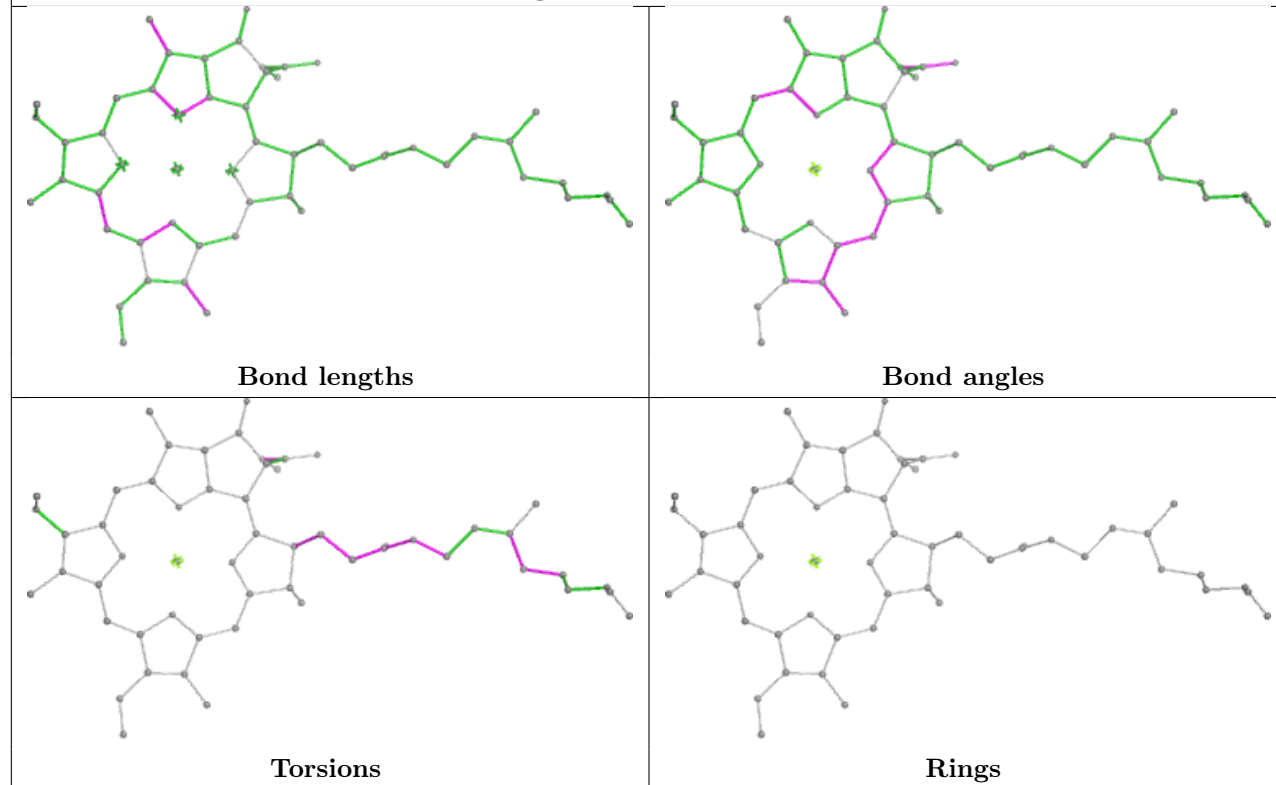




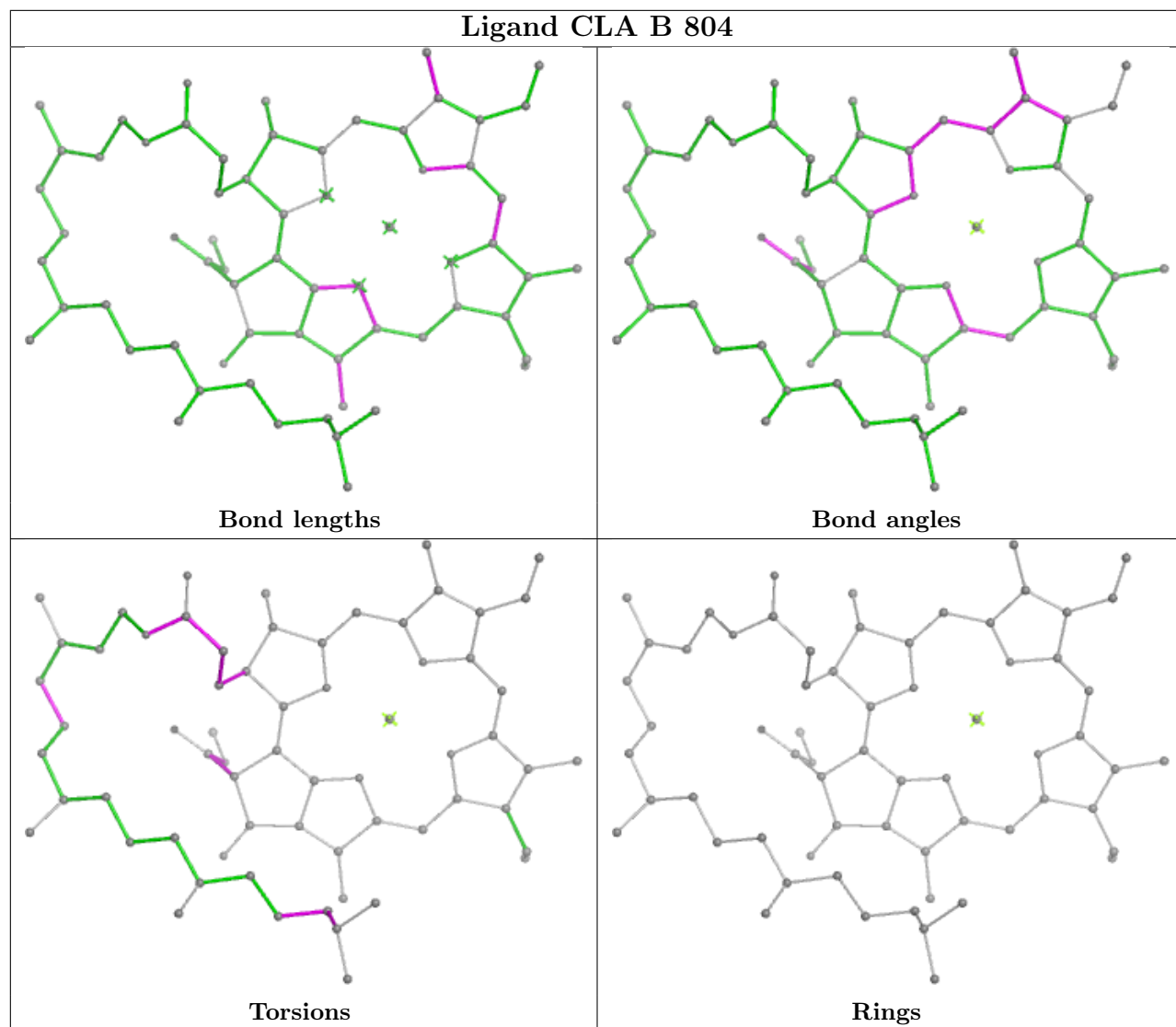




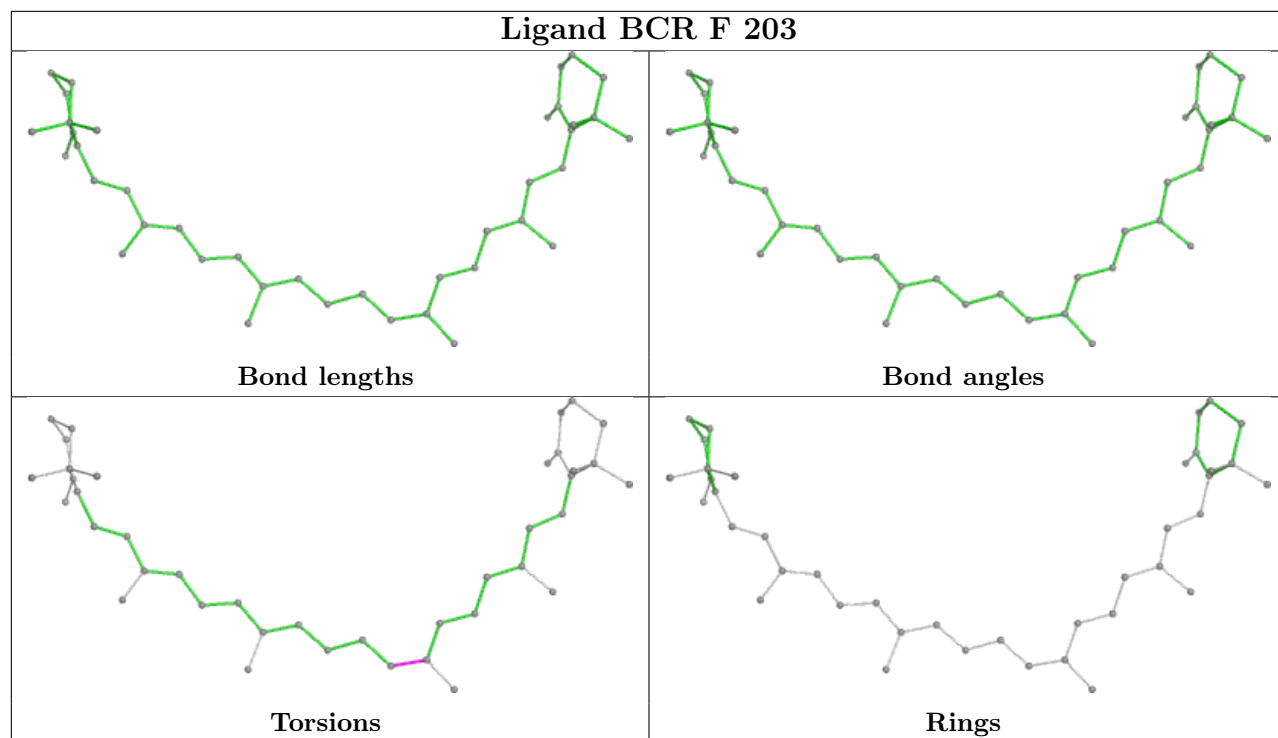


**Ligand CLA B 821****Ligand CLA N 838**



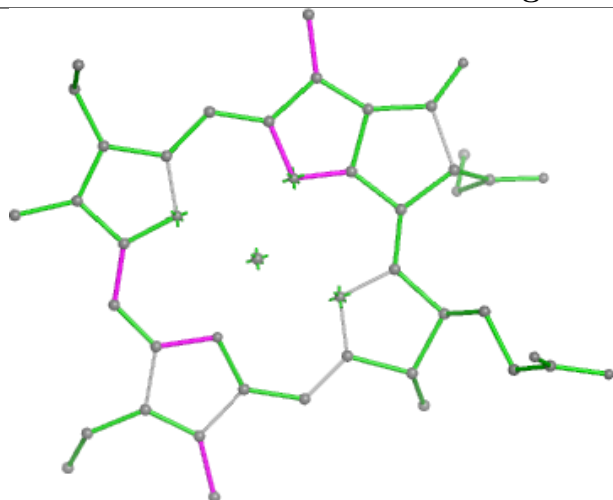




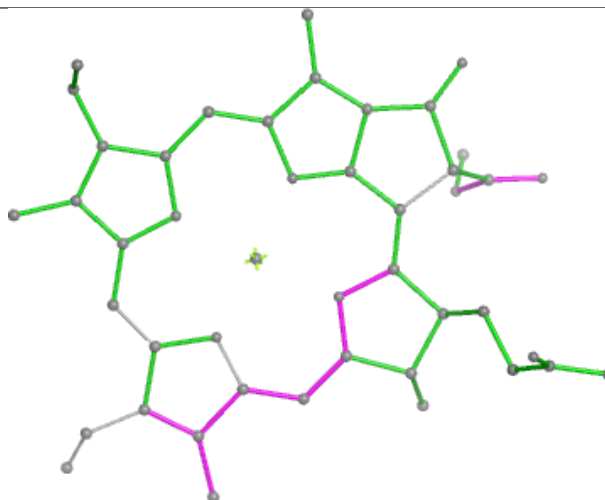




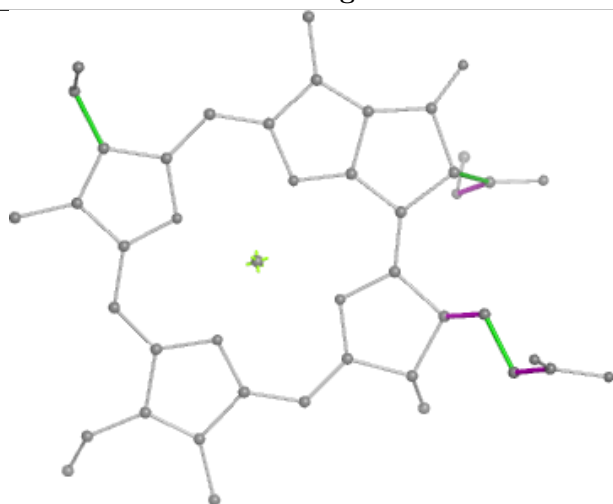
## Ligand CLA i 102



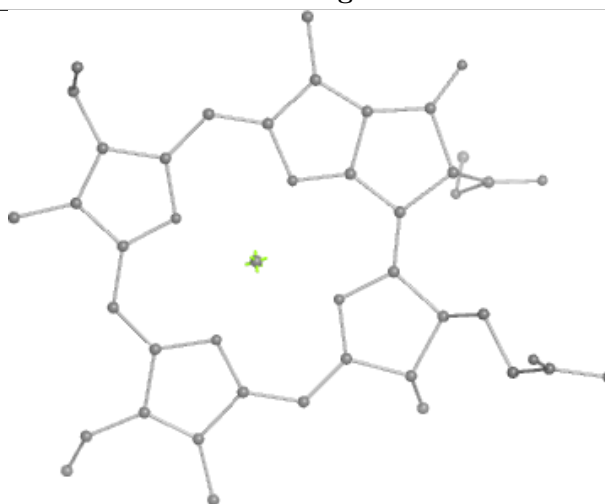
Bond lengths



Bond angles

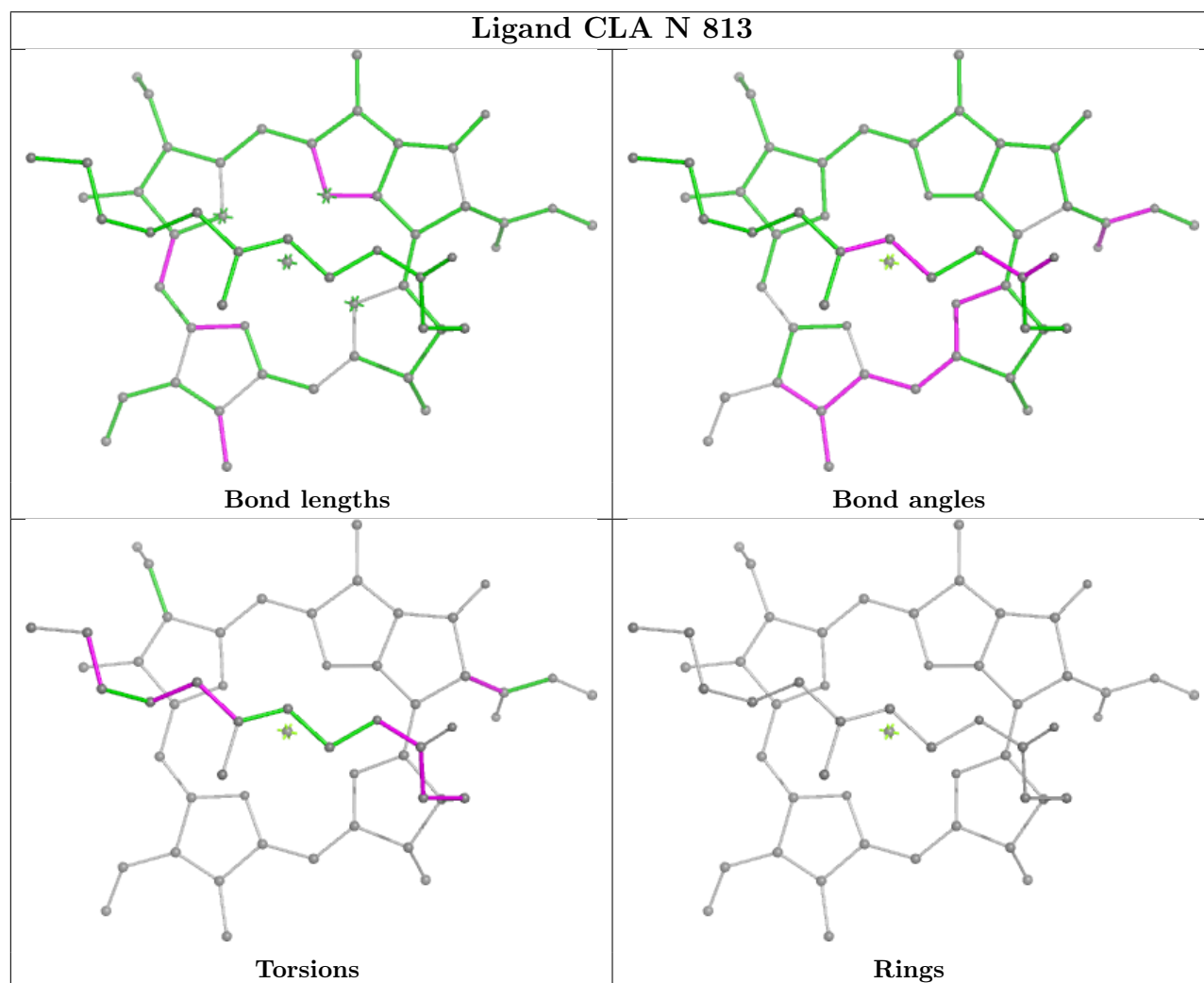
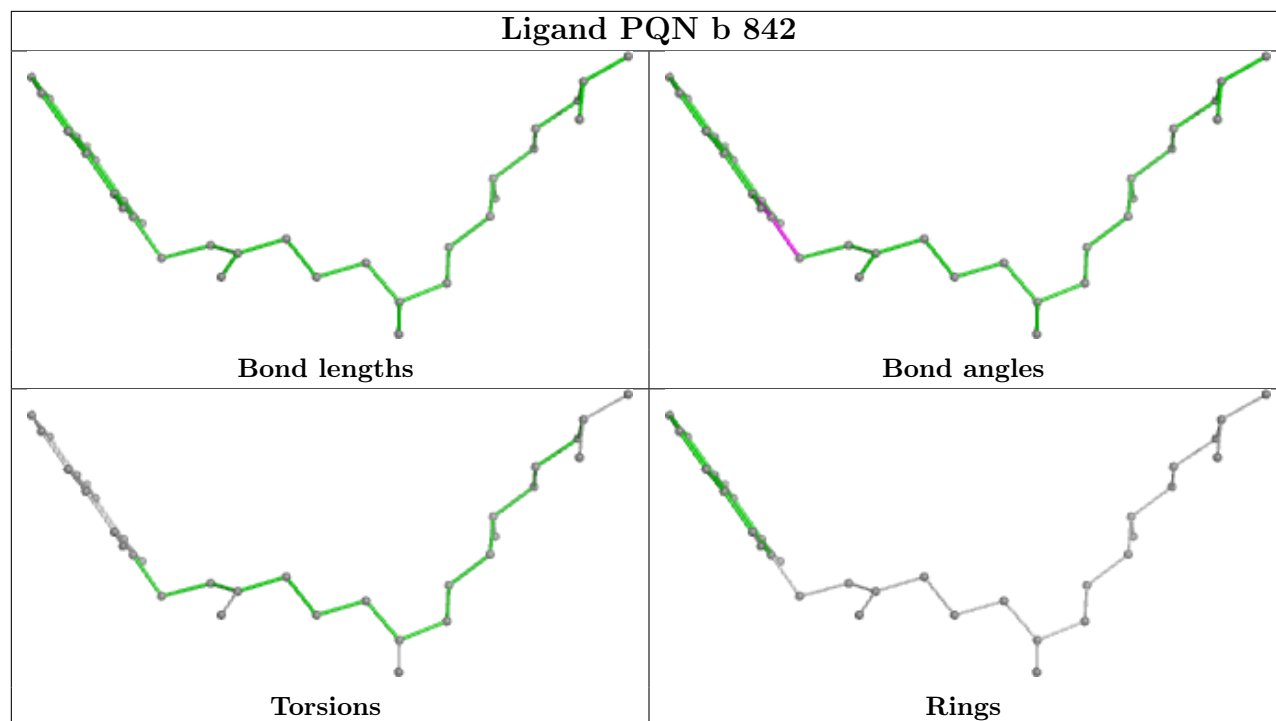


Torsions

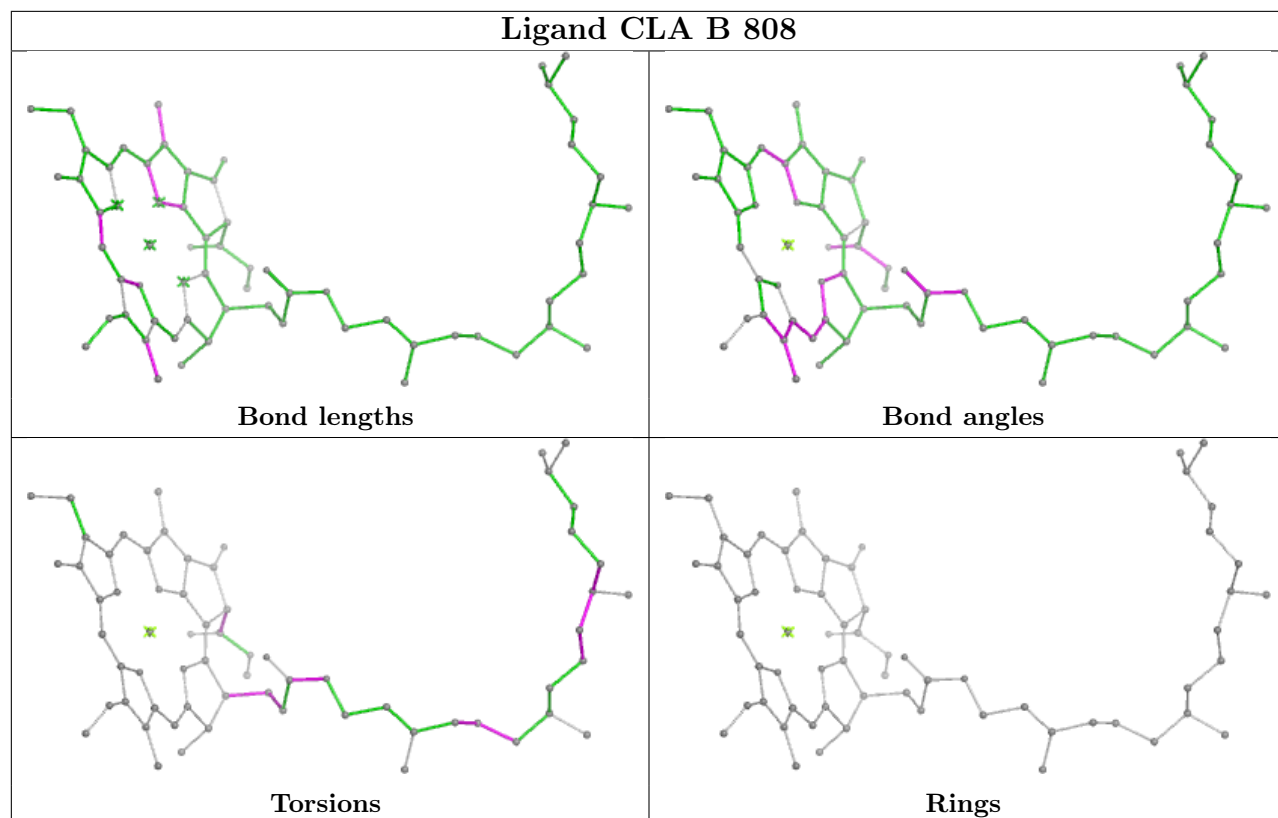


Rings



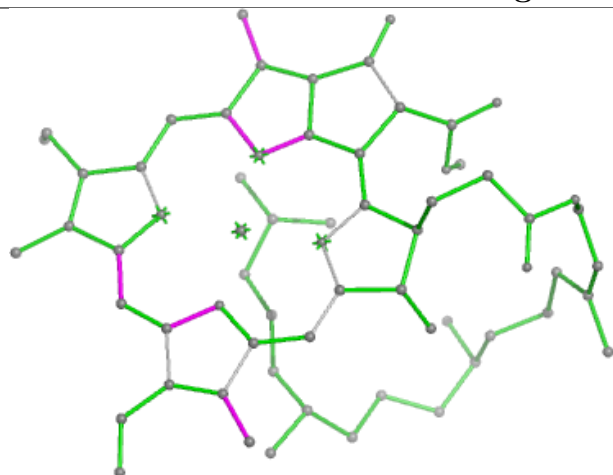




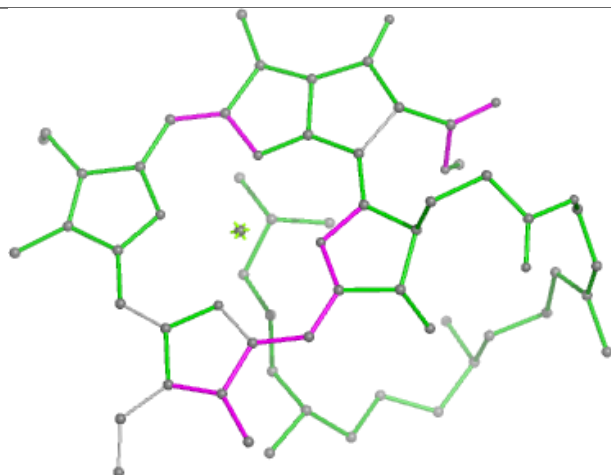




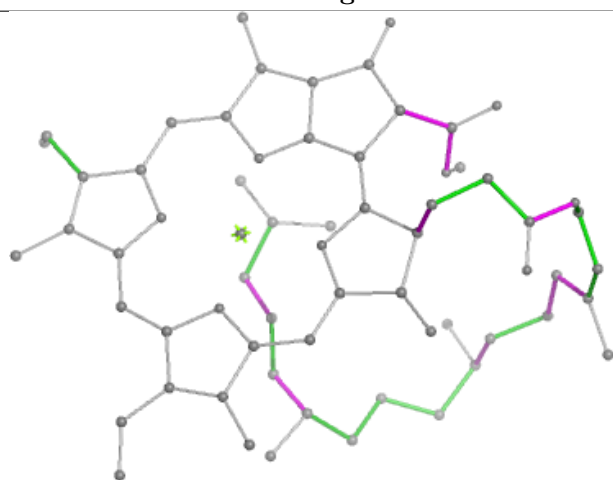
## Ligand CLA B 805



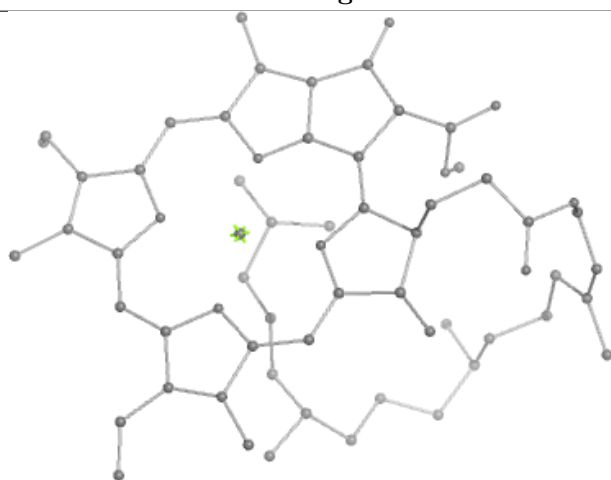
Bond lengths



Bond angles



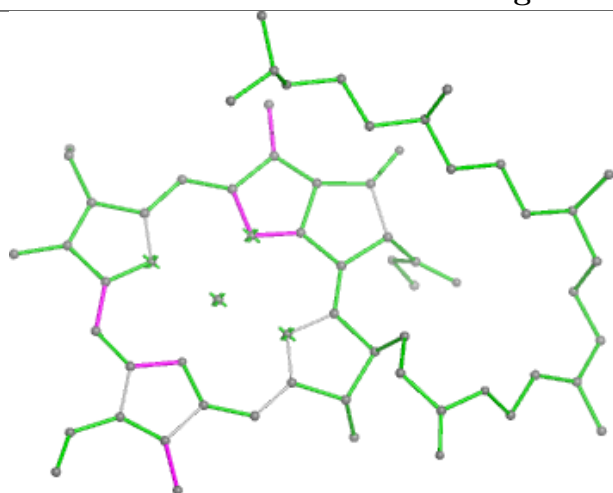
Torsions



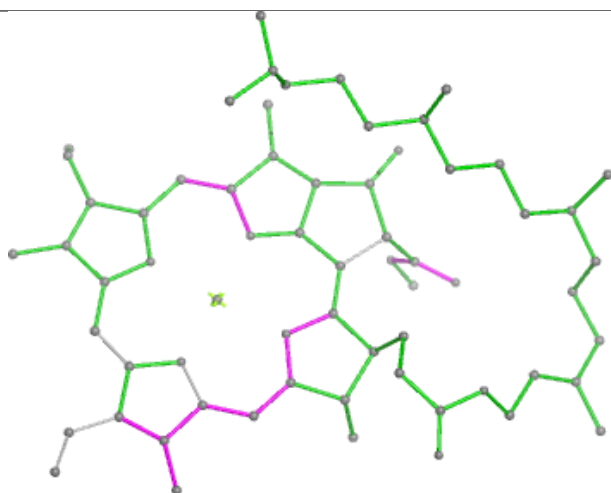
Rings



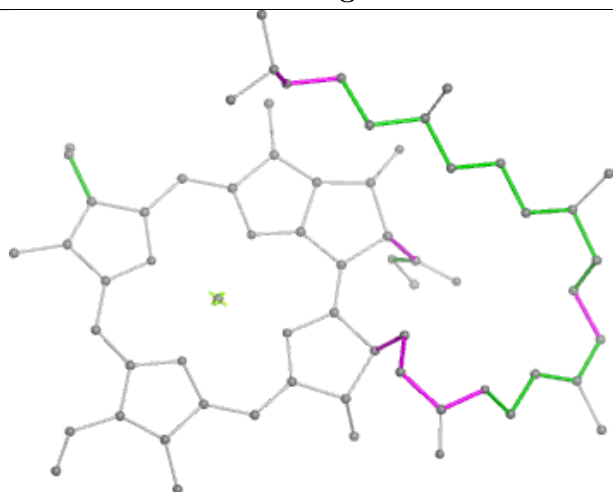
## Ligand CLA O 805



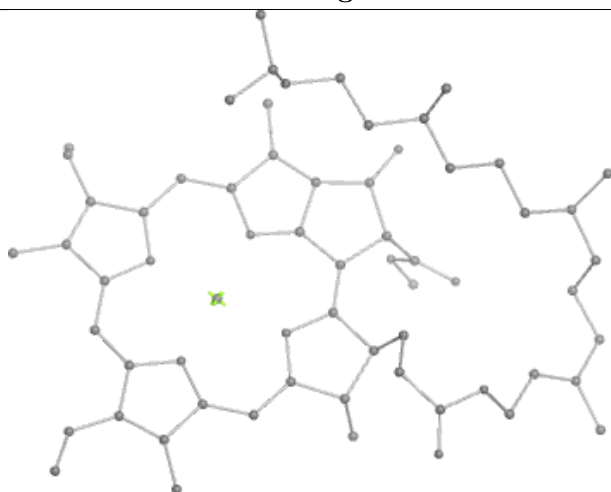
Bond lengths



Bond angles



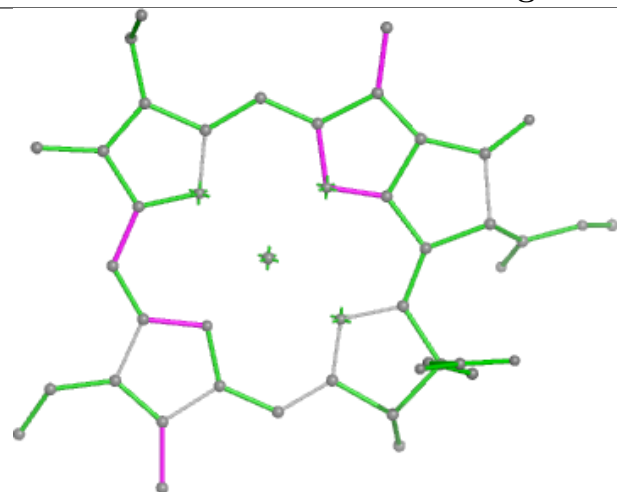
Torsions



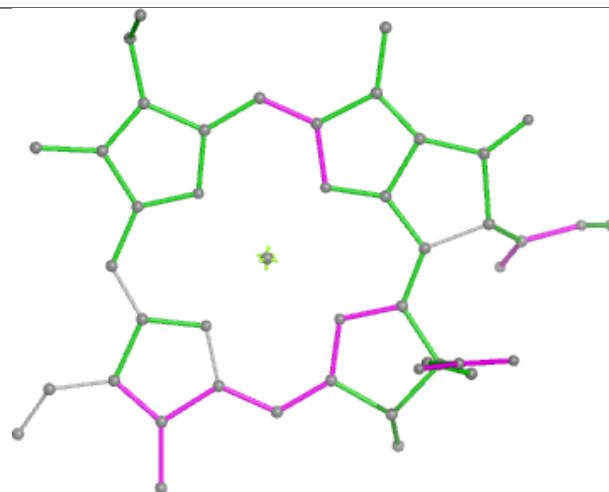
Rings



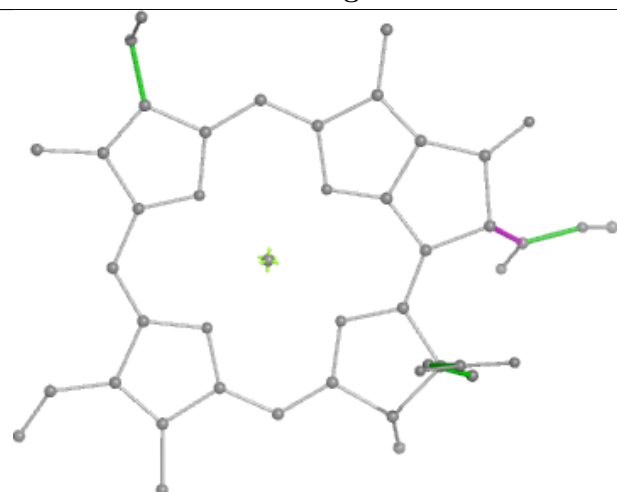
## Ligand CLA A 808



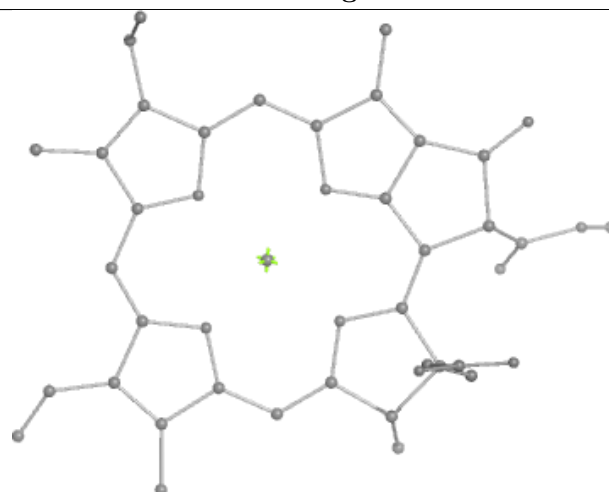
Bond lengths



Bond angles

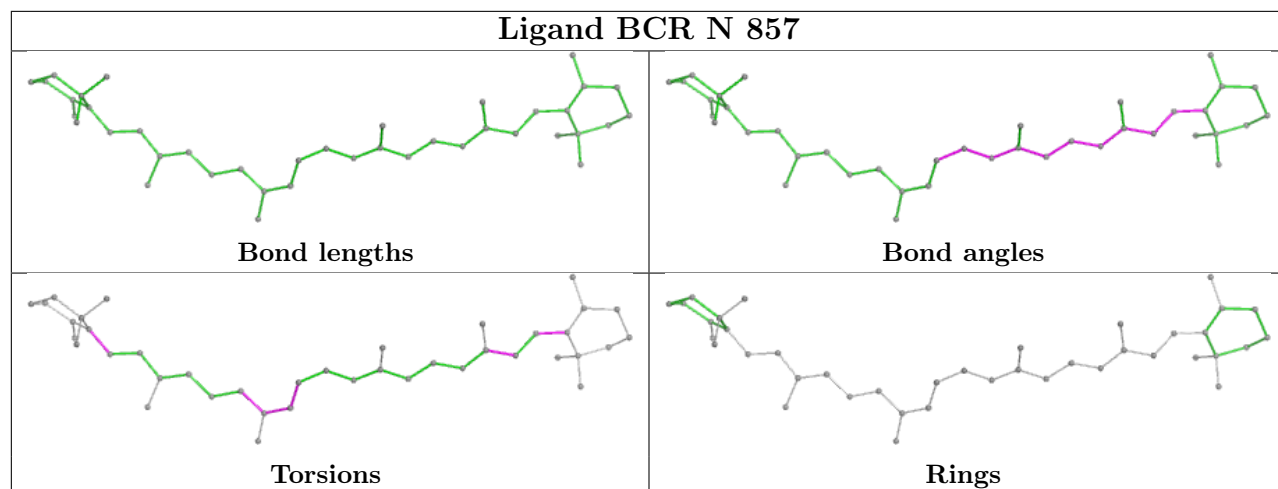
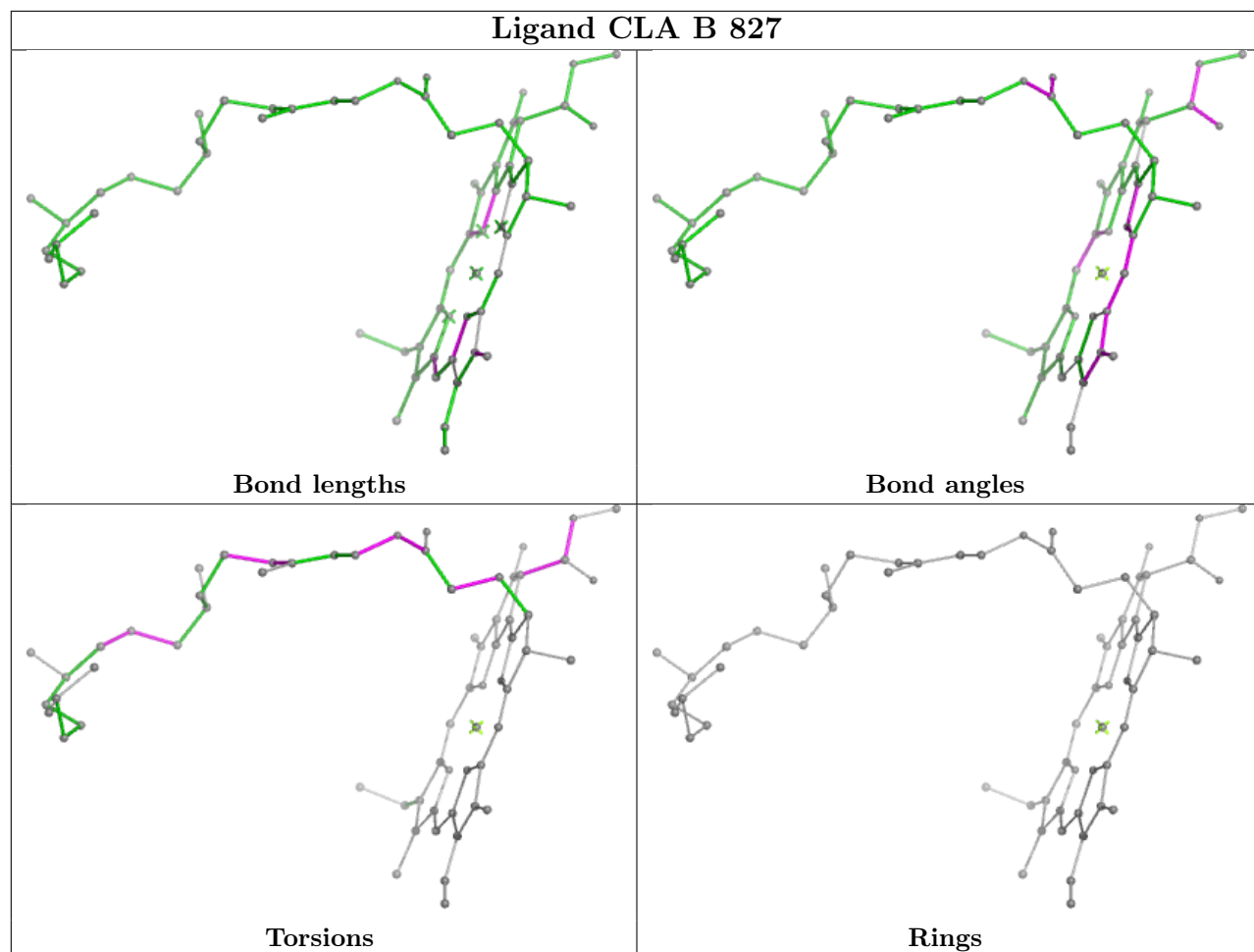


Torsions

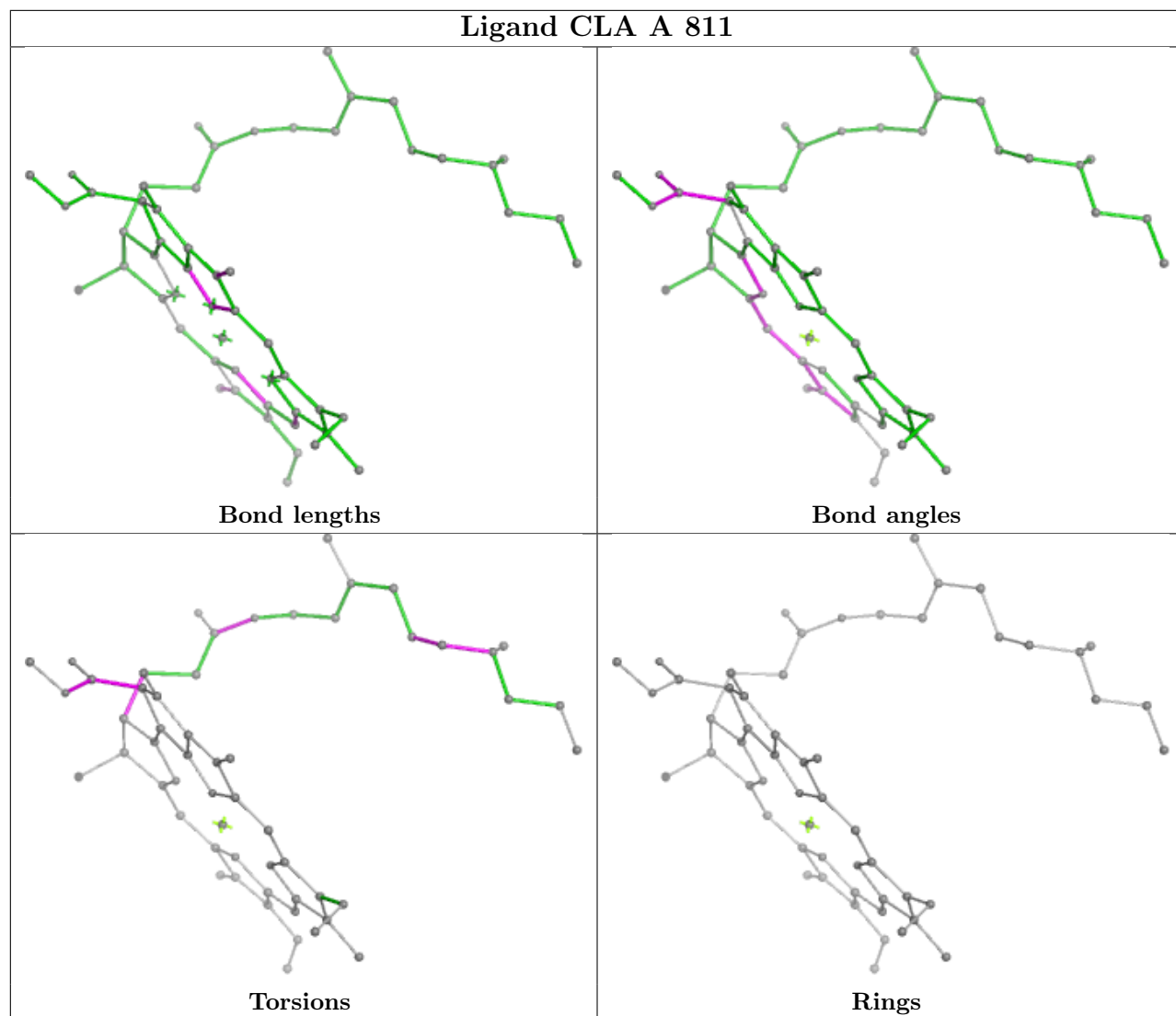


Rings



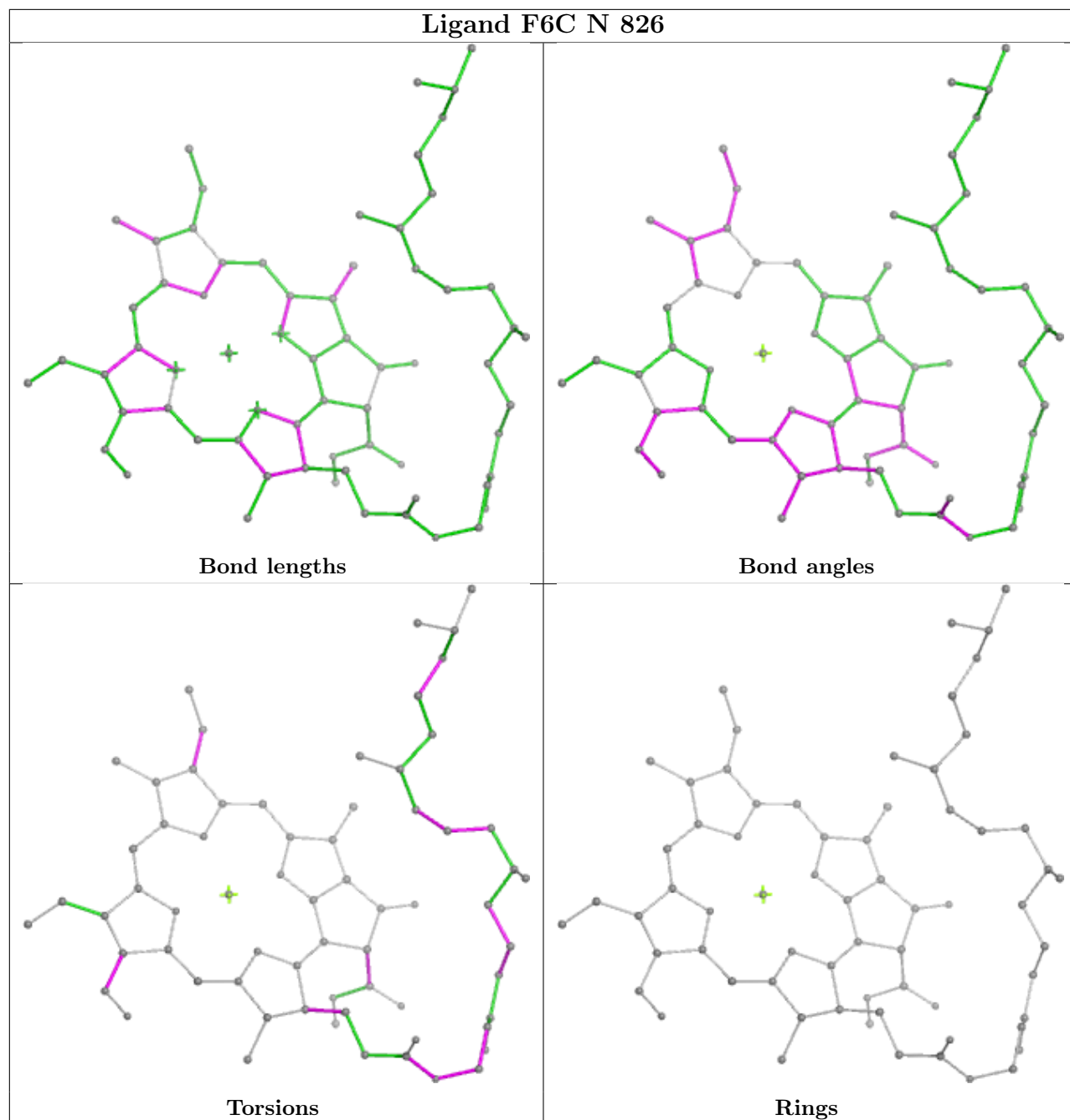






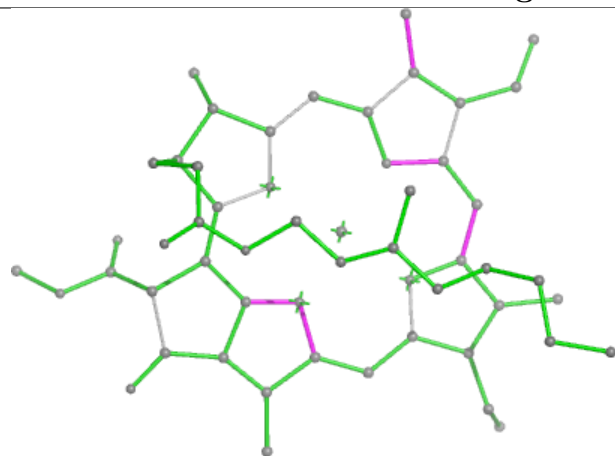


## Ligand F6C N 826

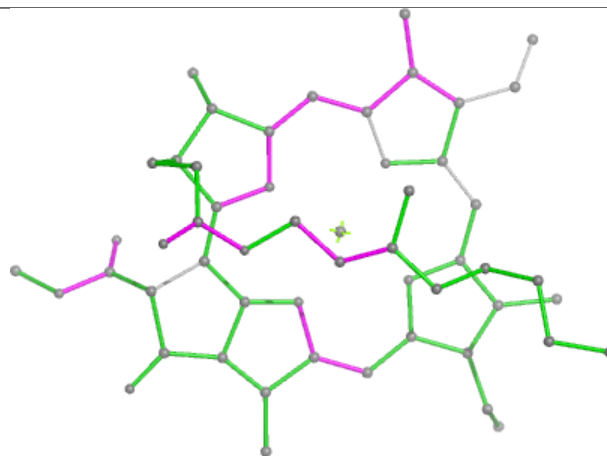




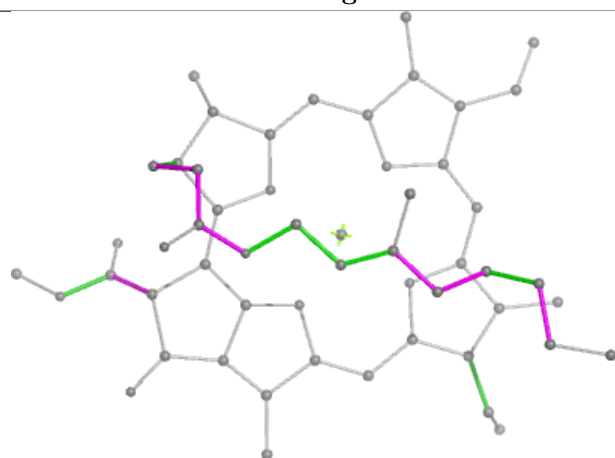
## Ligand CLA A 813



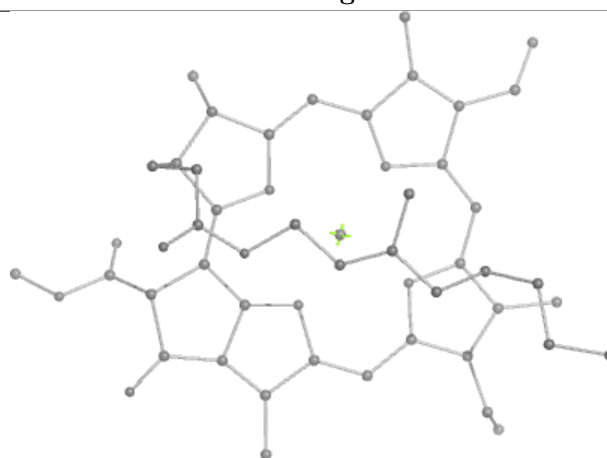
Bond lengths



Bond angles



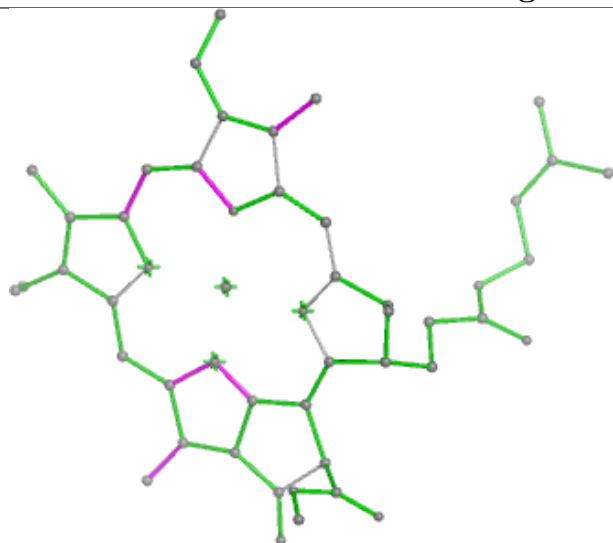
Torsions



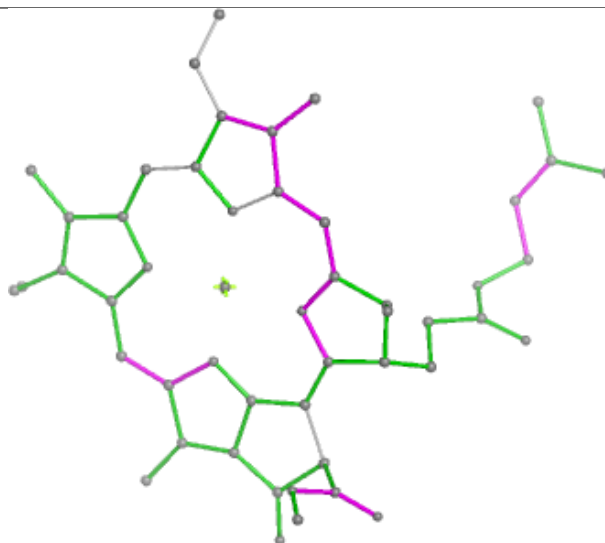
Rings



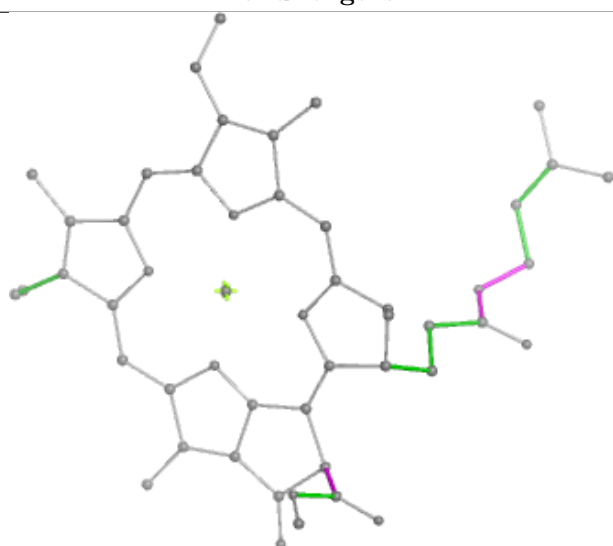
## Ligand CLA a 832



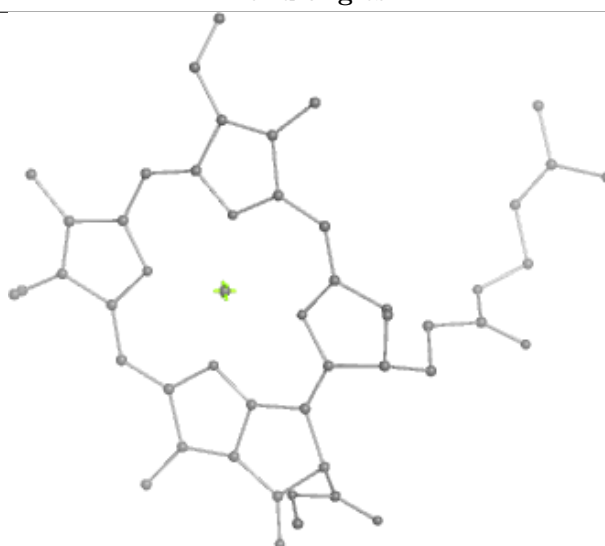
Bond lengths



Bond angles

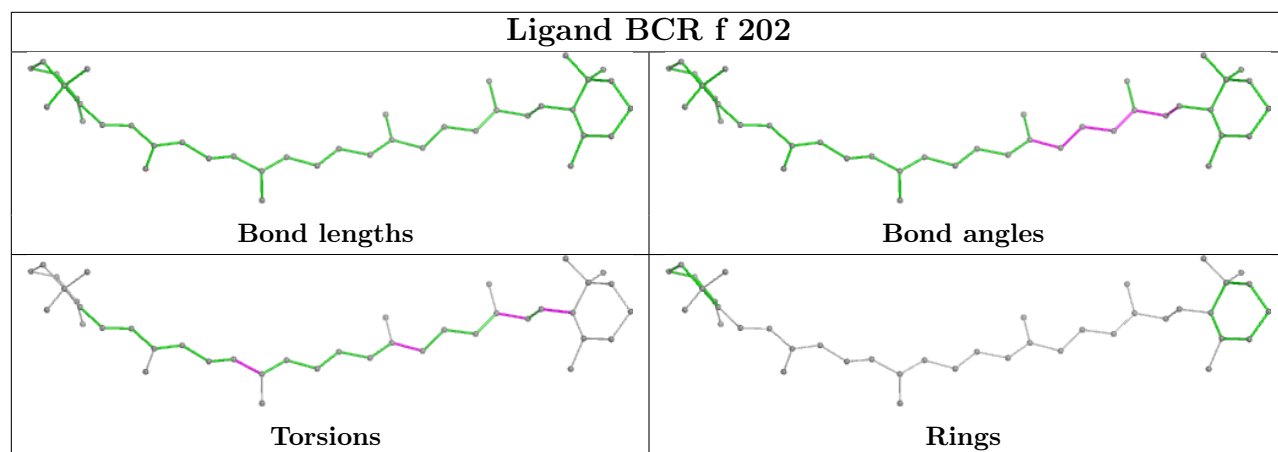
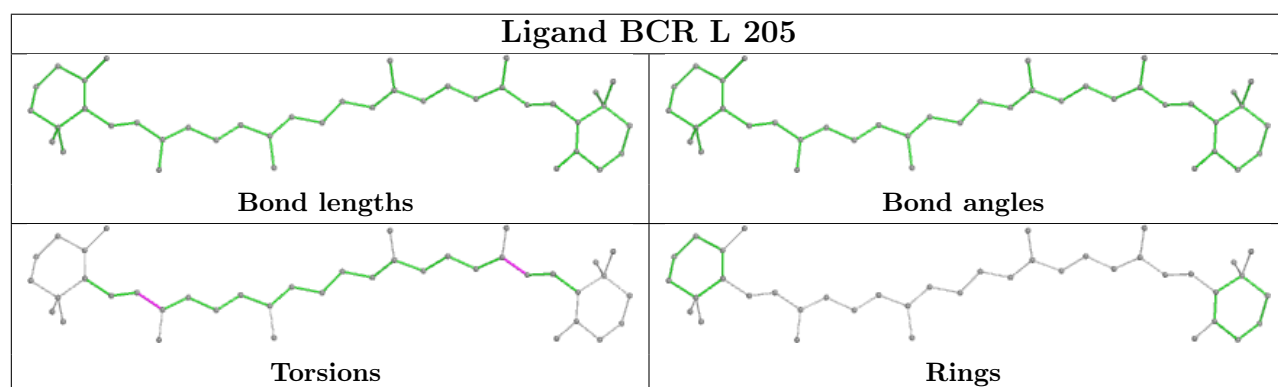
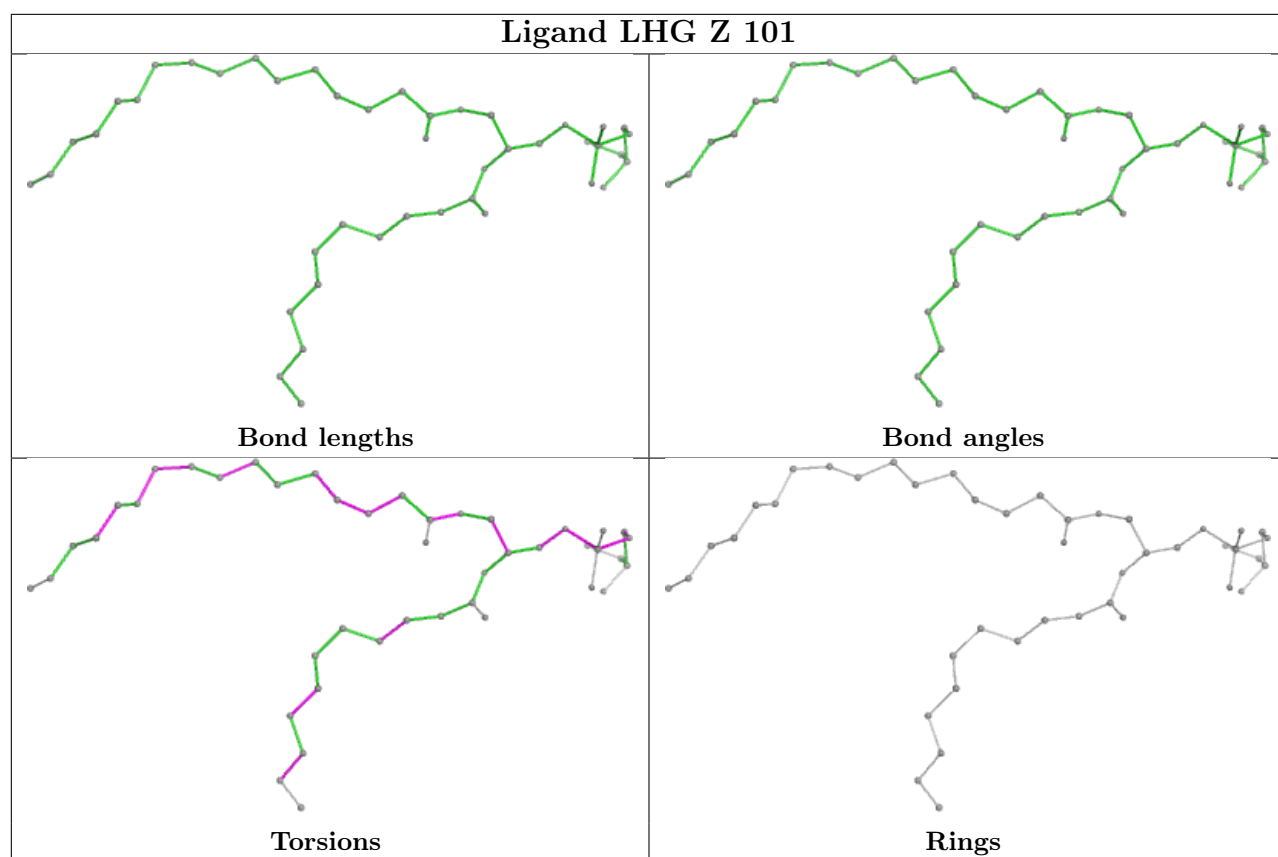


Torsions



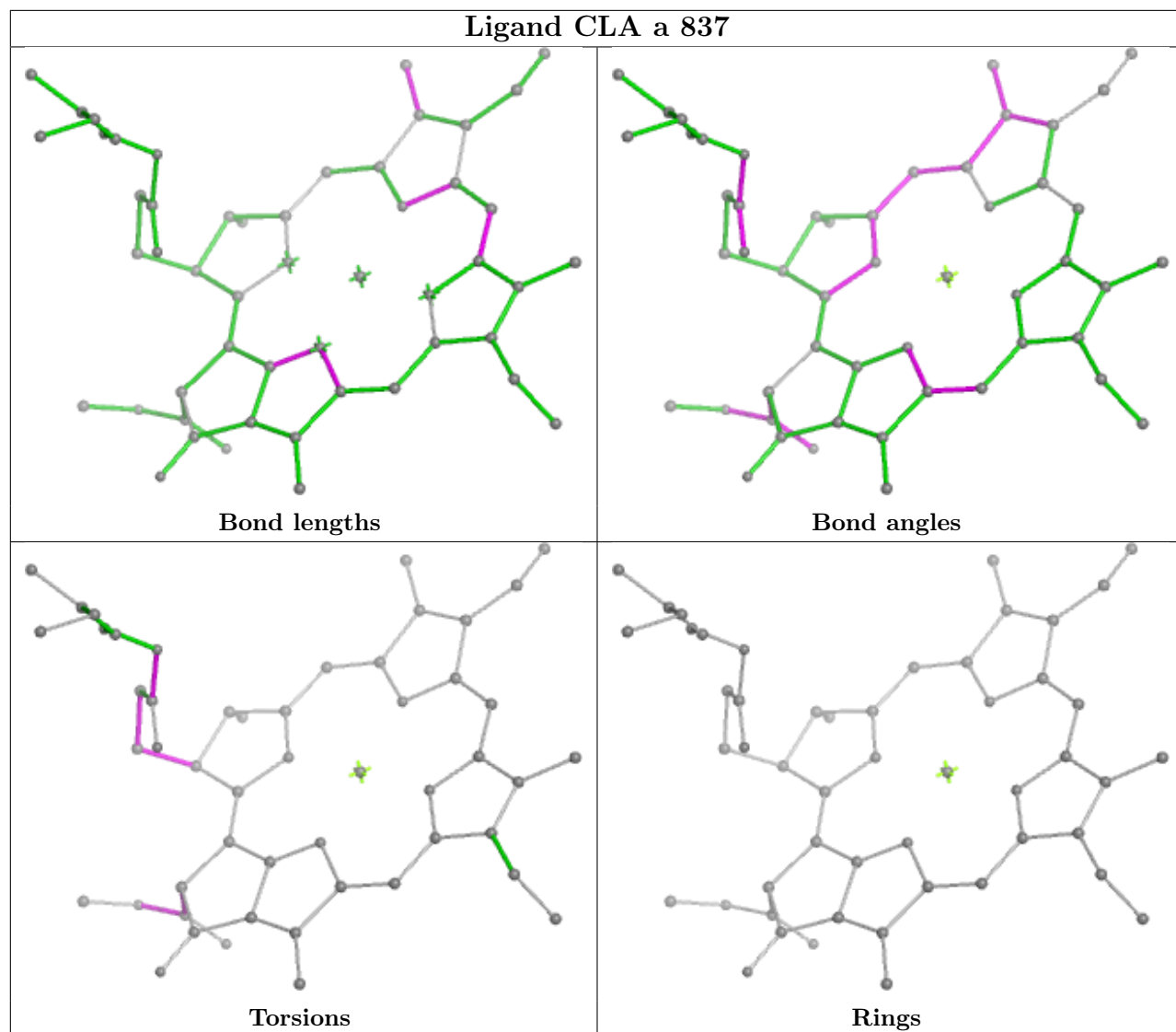
Rings



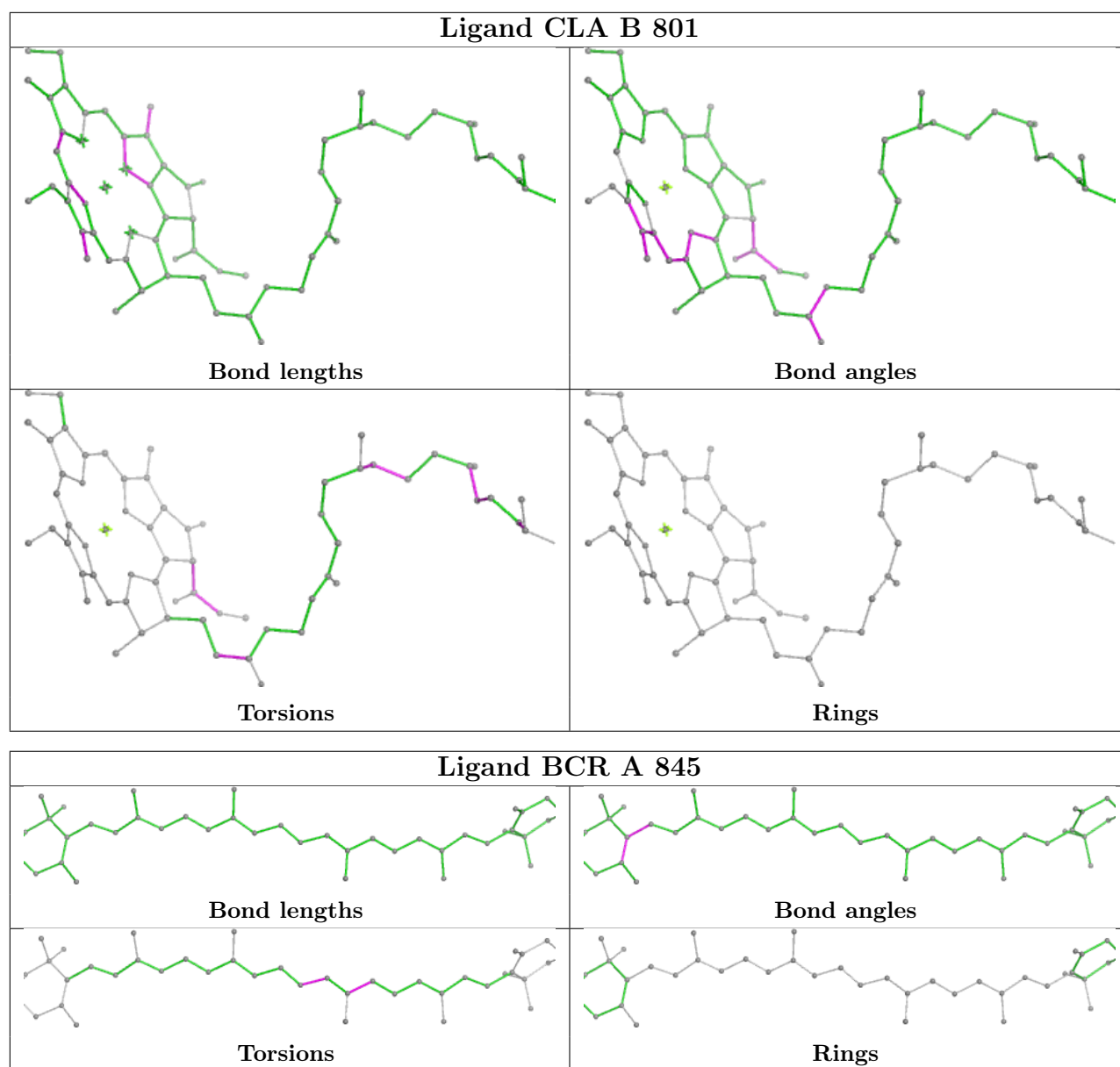




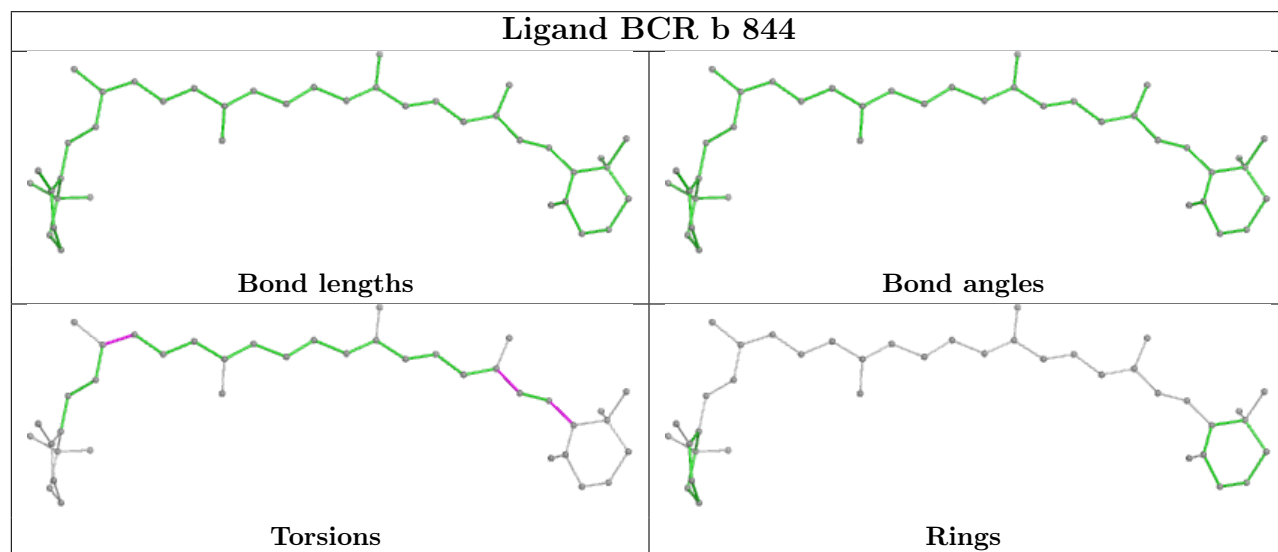
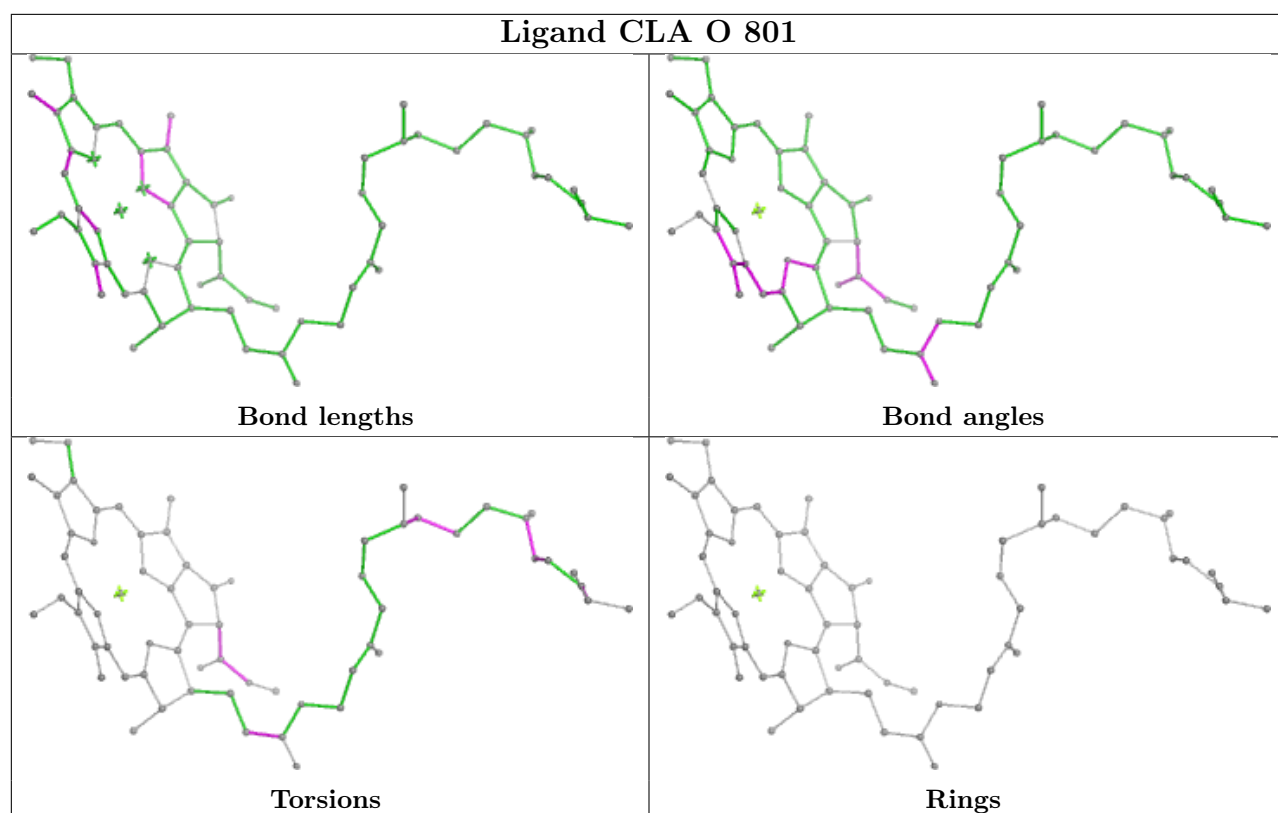
## Ligand CLA a 837



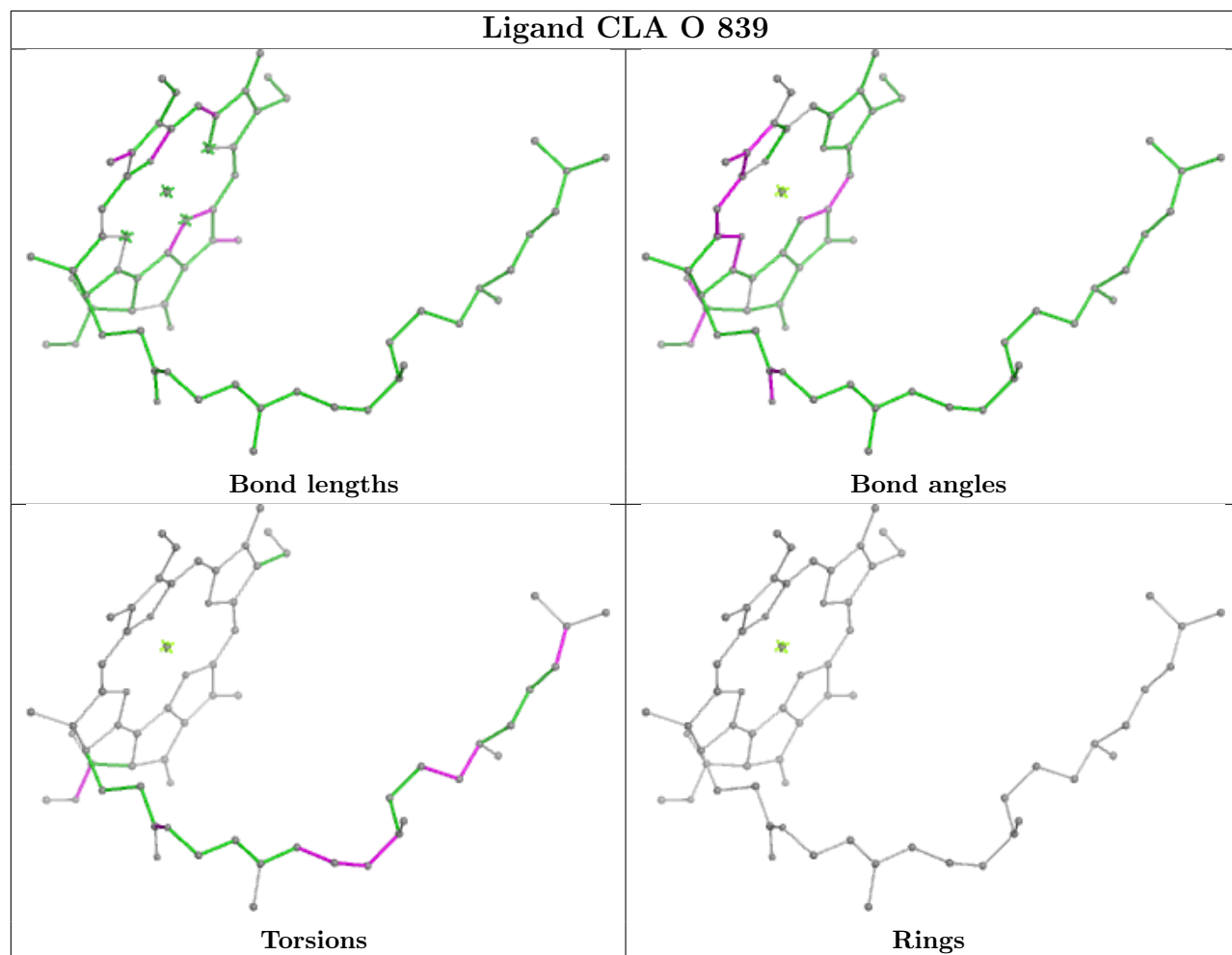




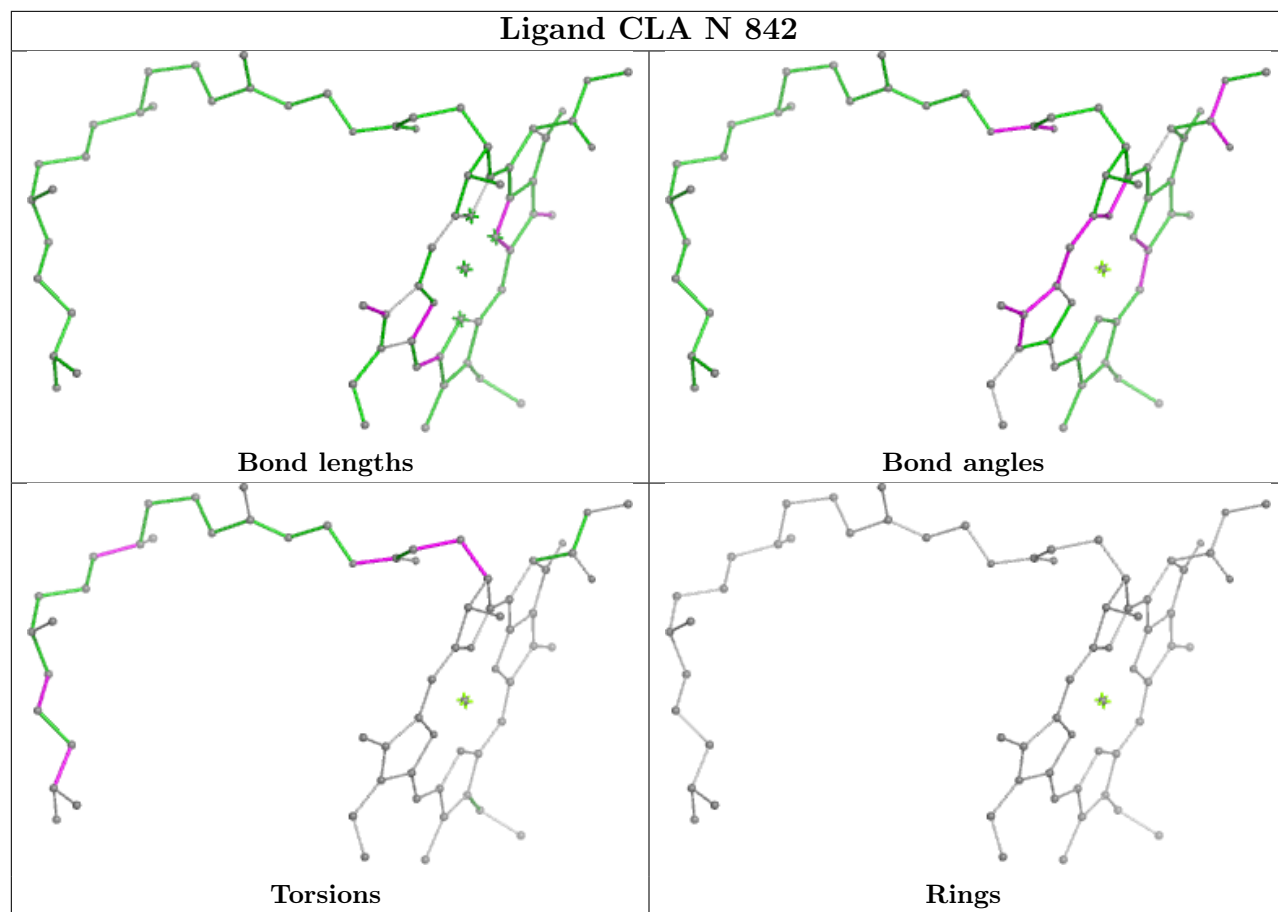






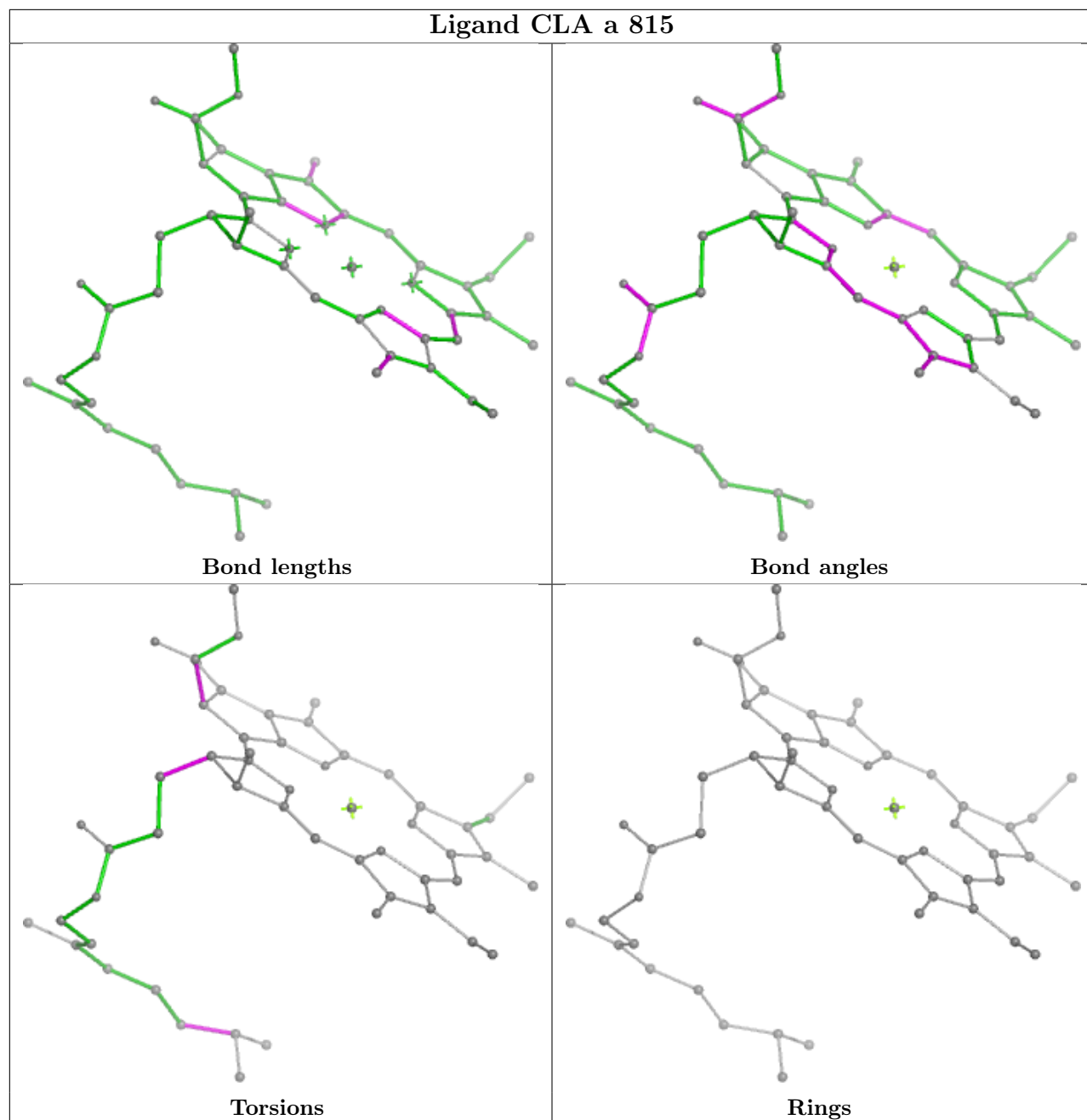






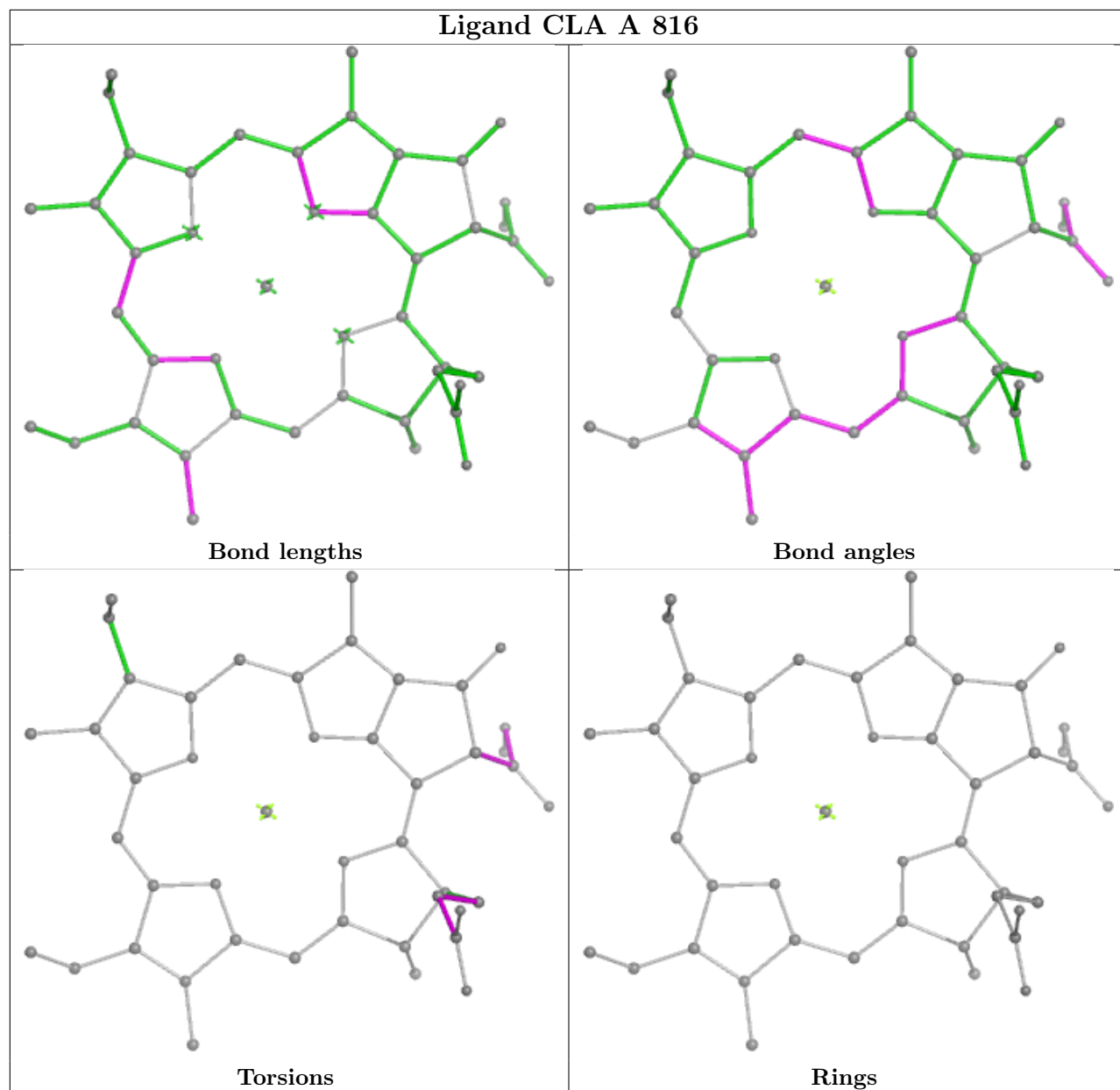


## Ligand CLA a 815

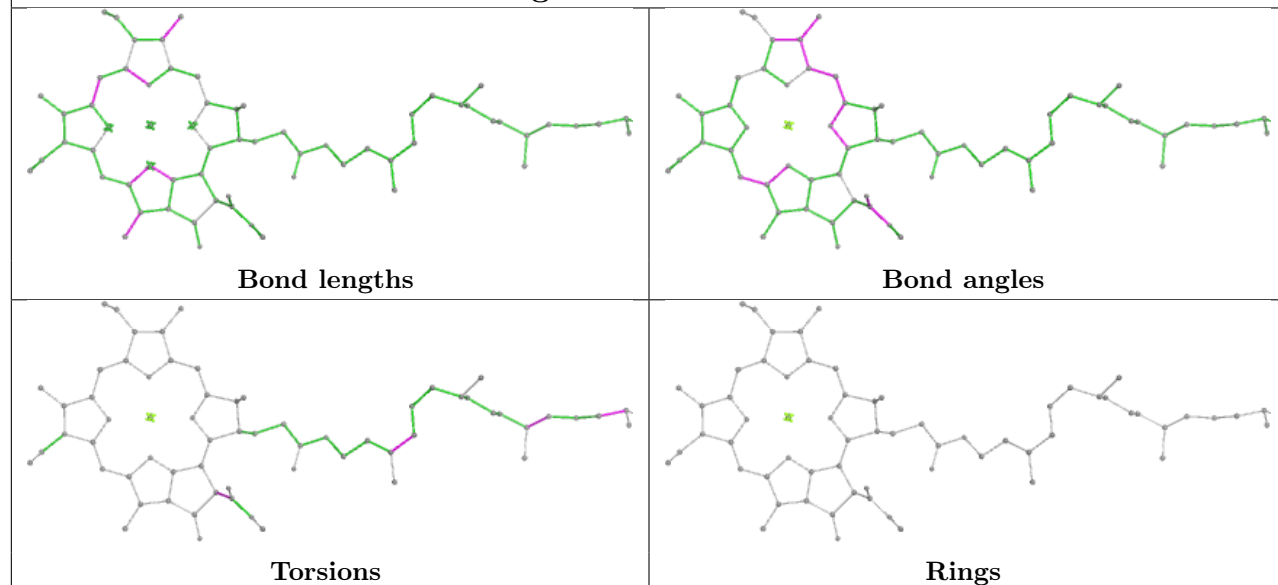
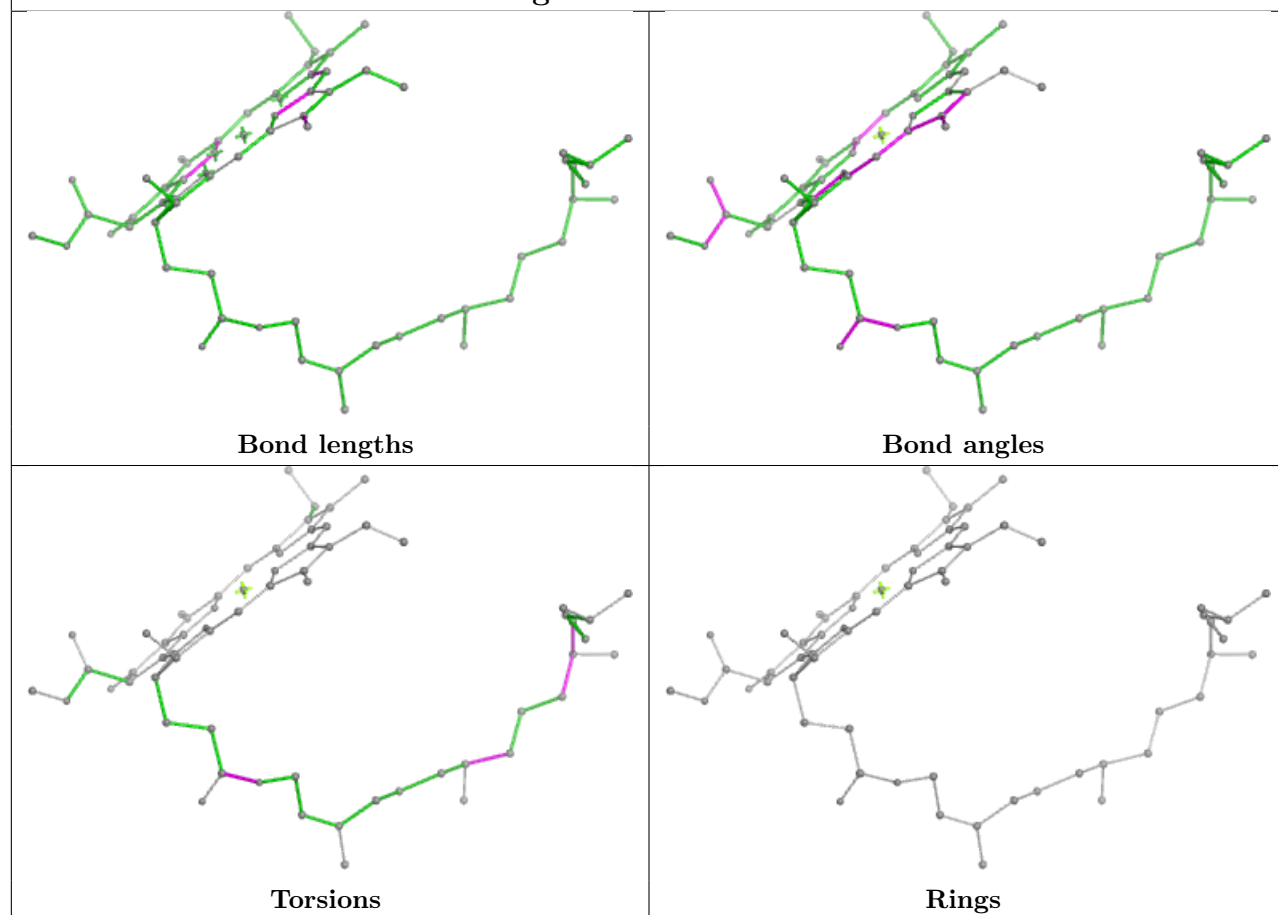




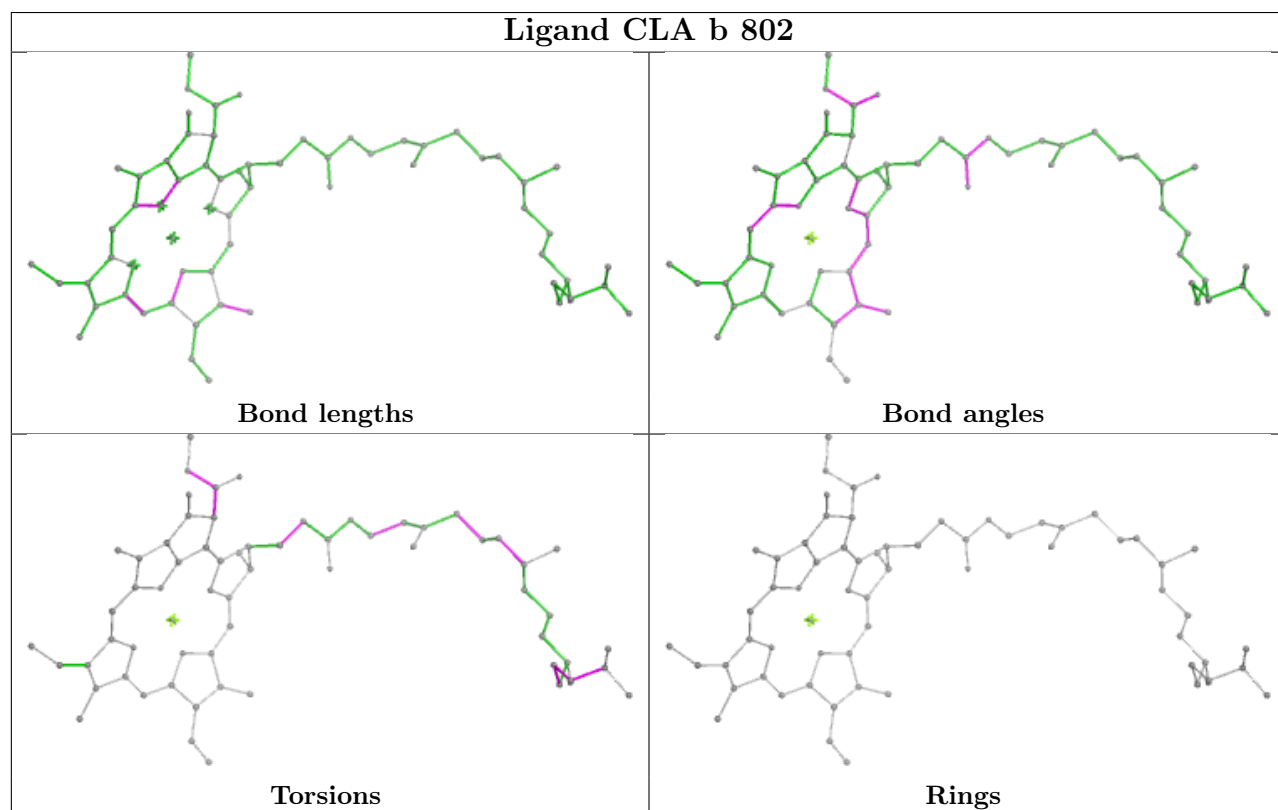
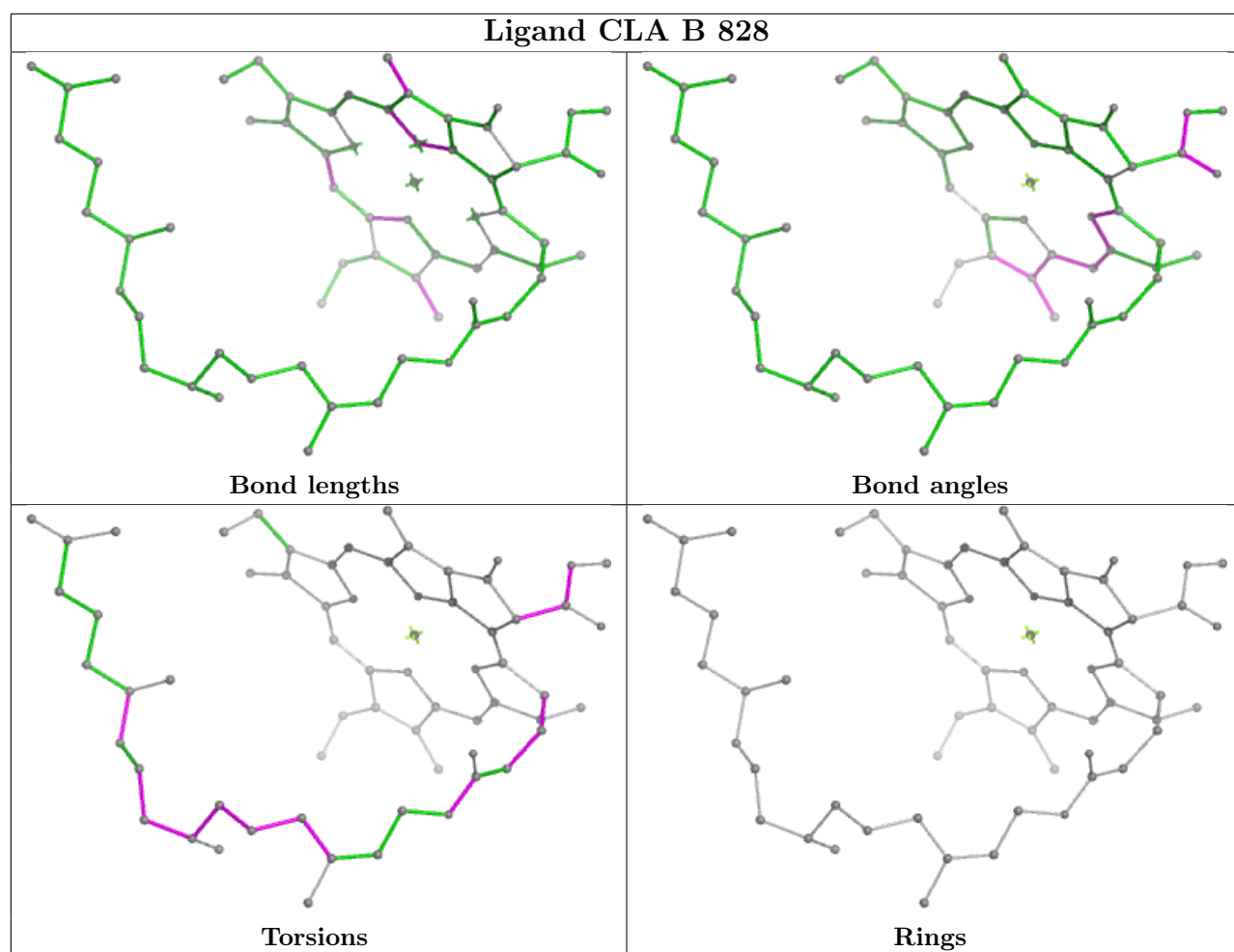
## Ligand CLA A 816





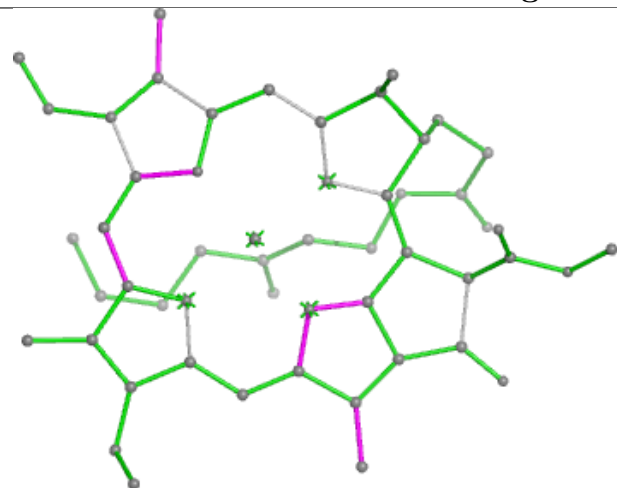
**Ligand CLA A 834****Ligand CLA B 817**



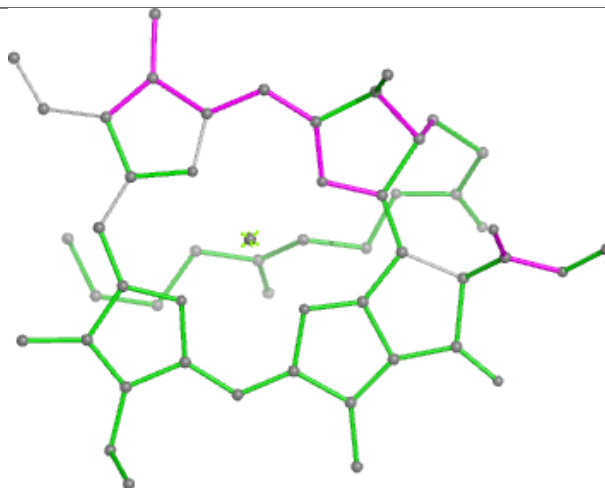




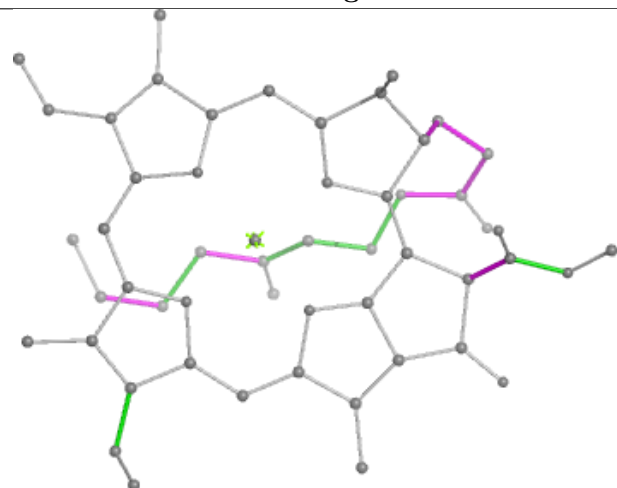
## Ligand CLA b 822



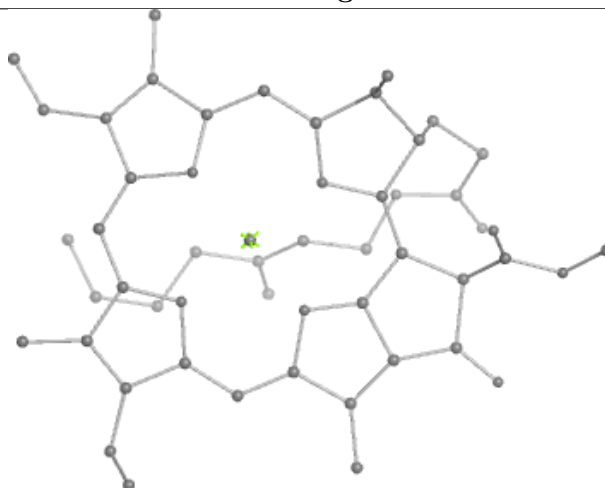
Bond lengths



Bond angles



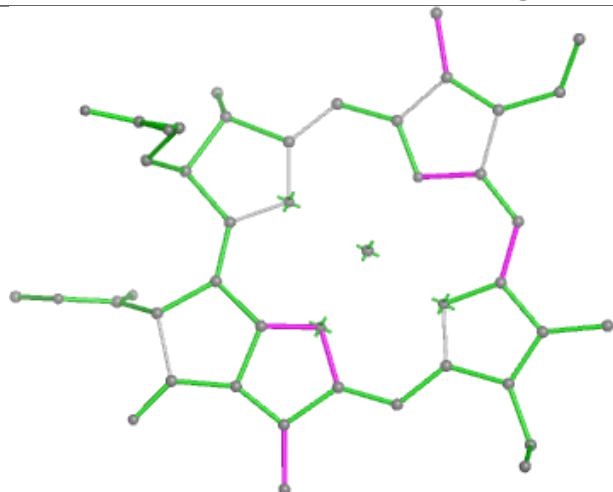
Torsions



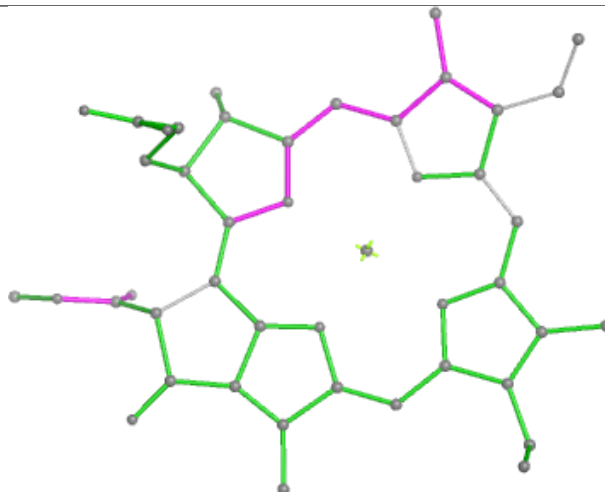
Rings



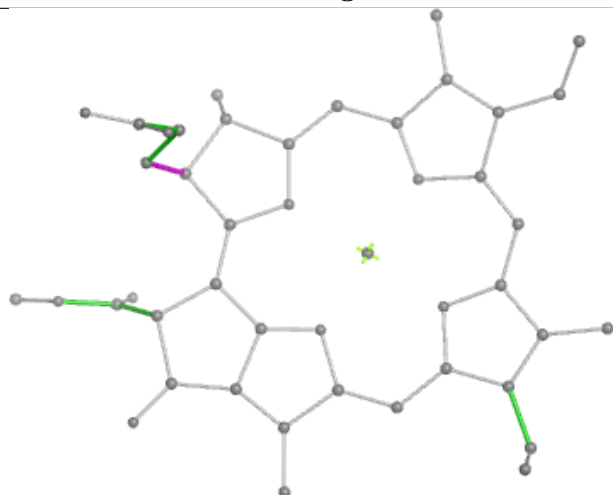
## Ligand CLA B 833



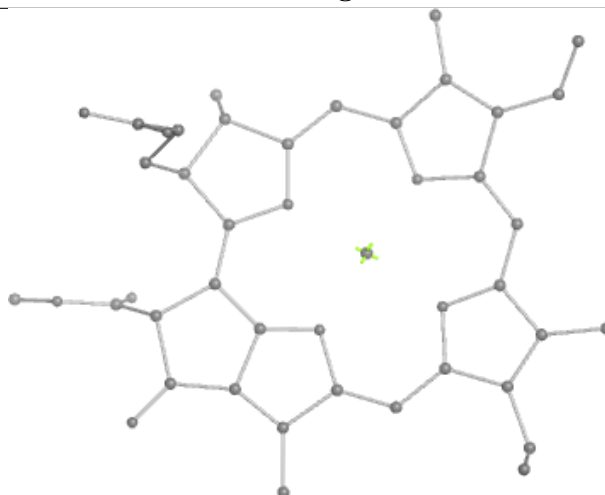
Bond lengths



Bond angles

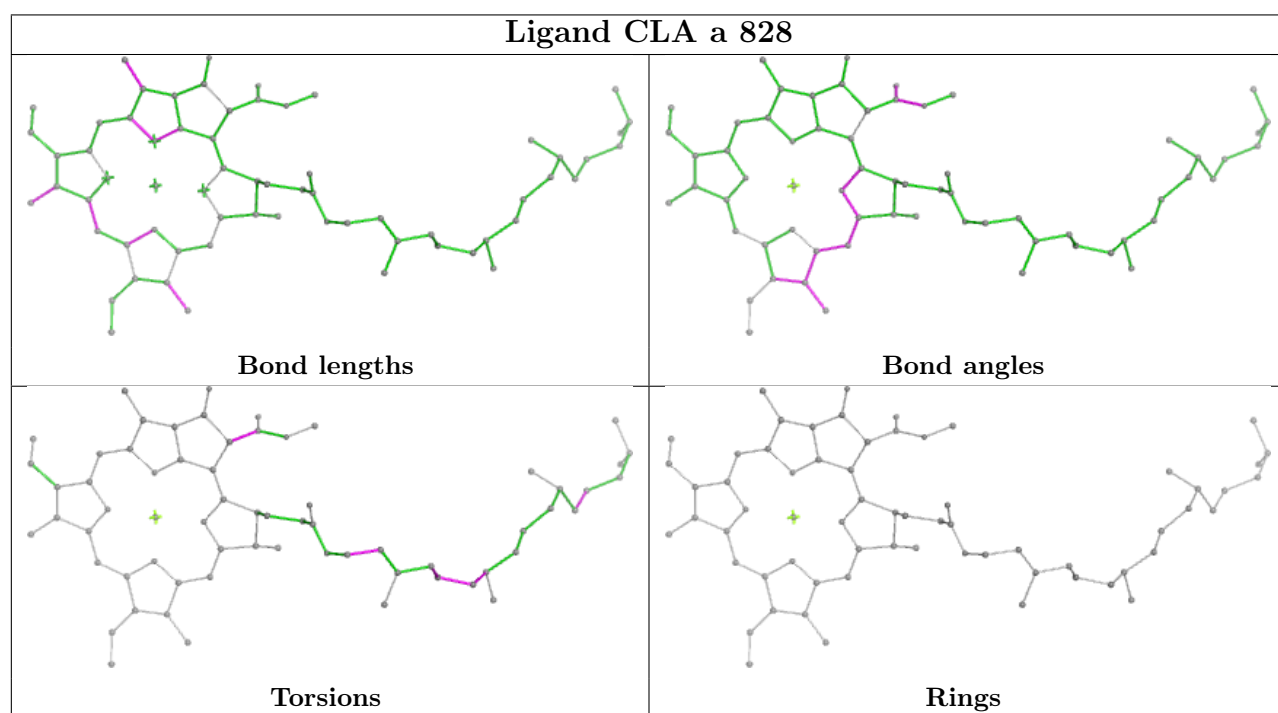
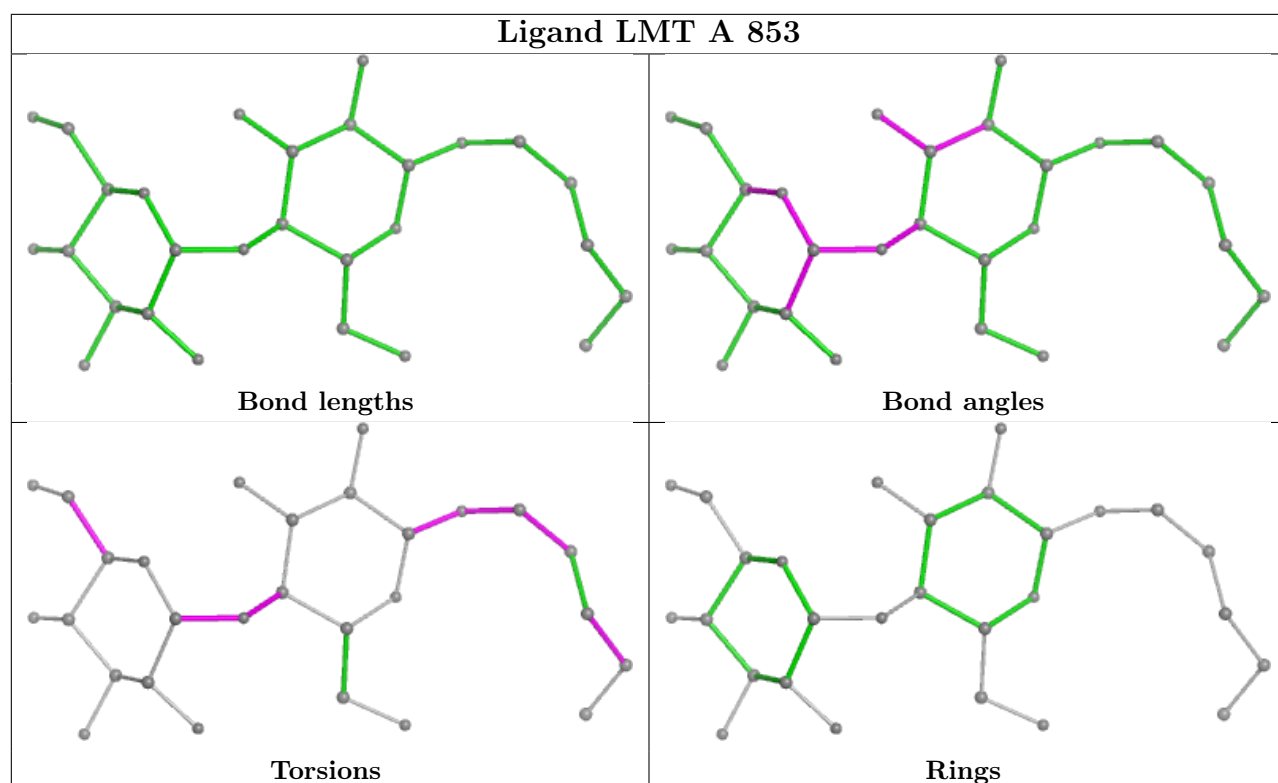


Torsions

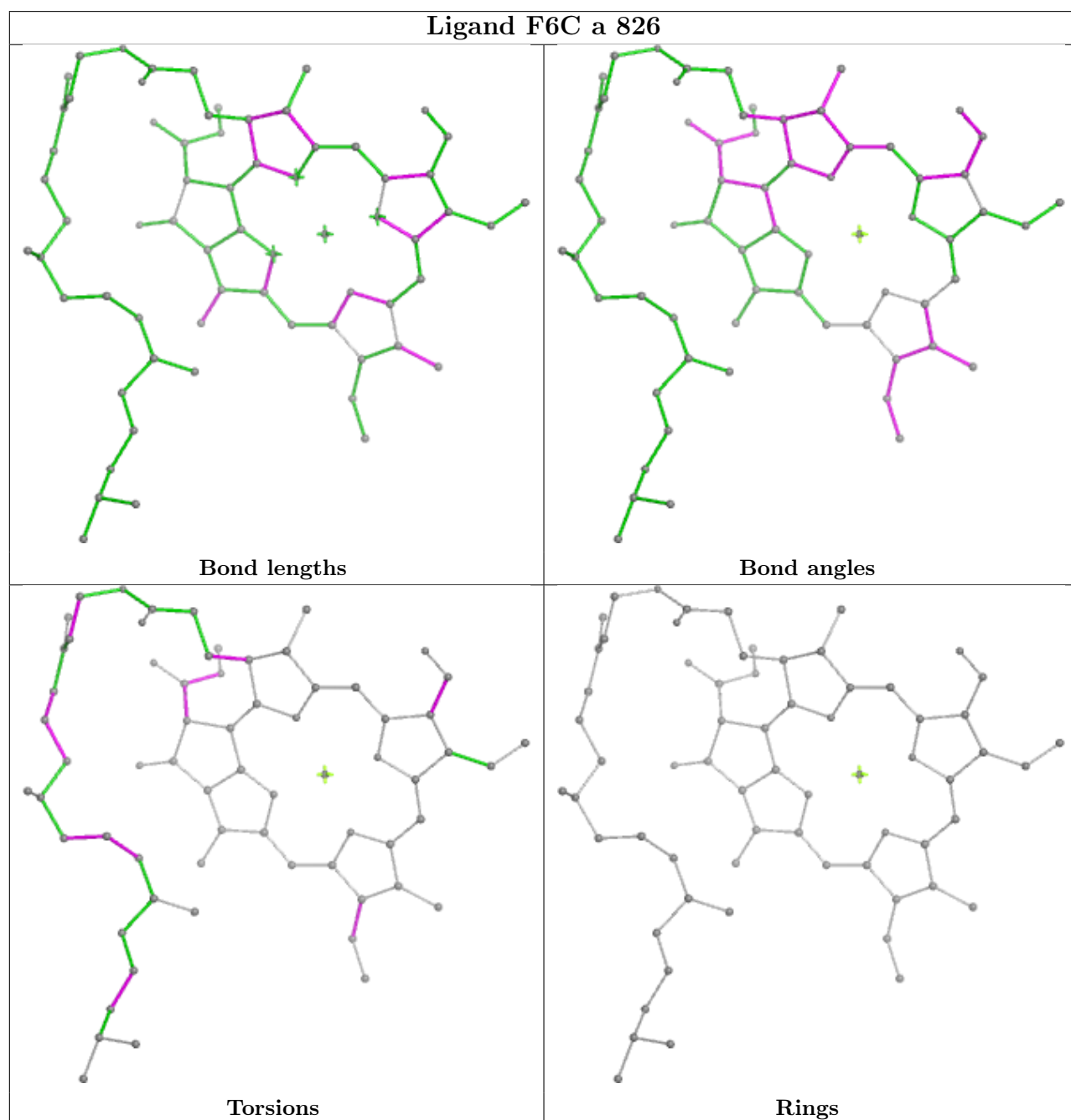
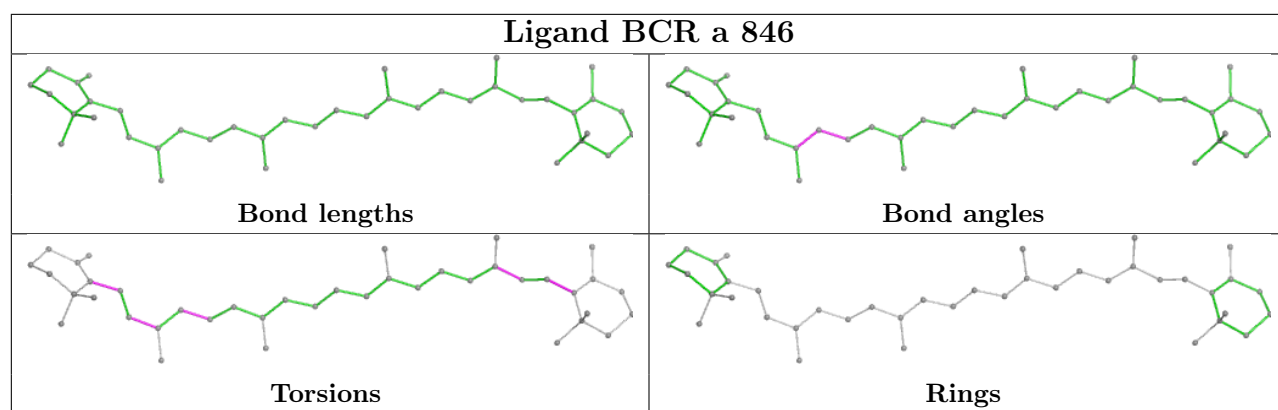


Rings

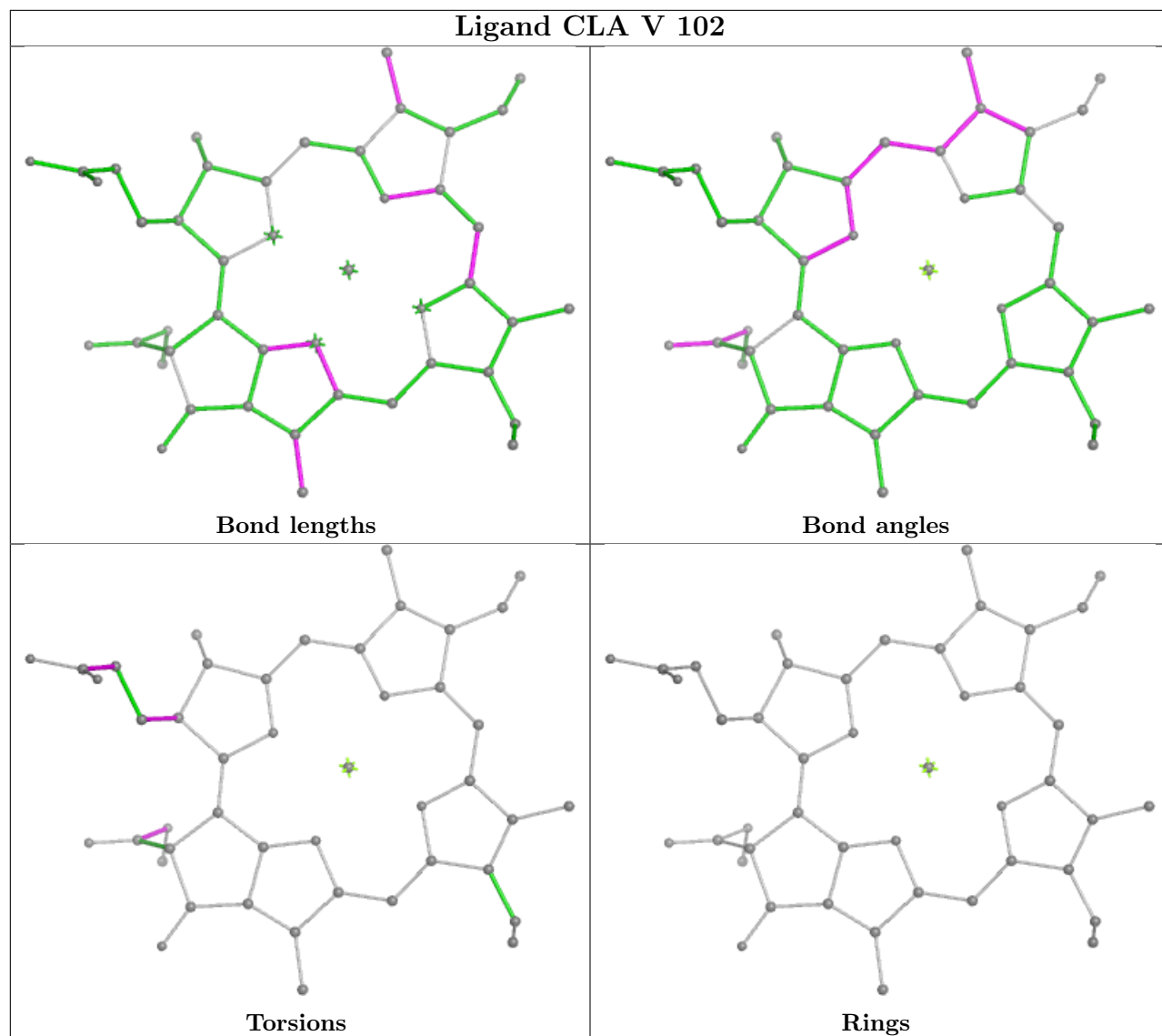




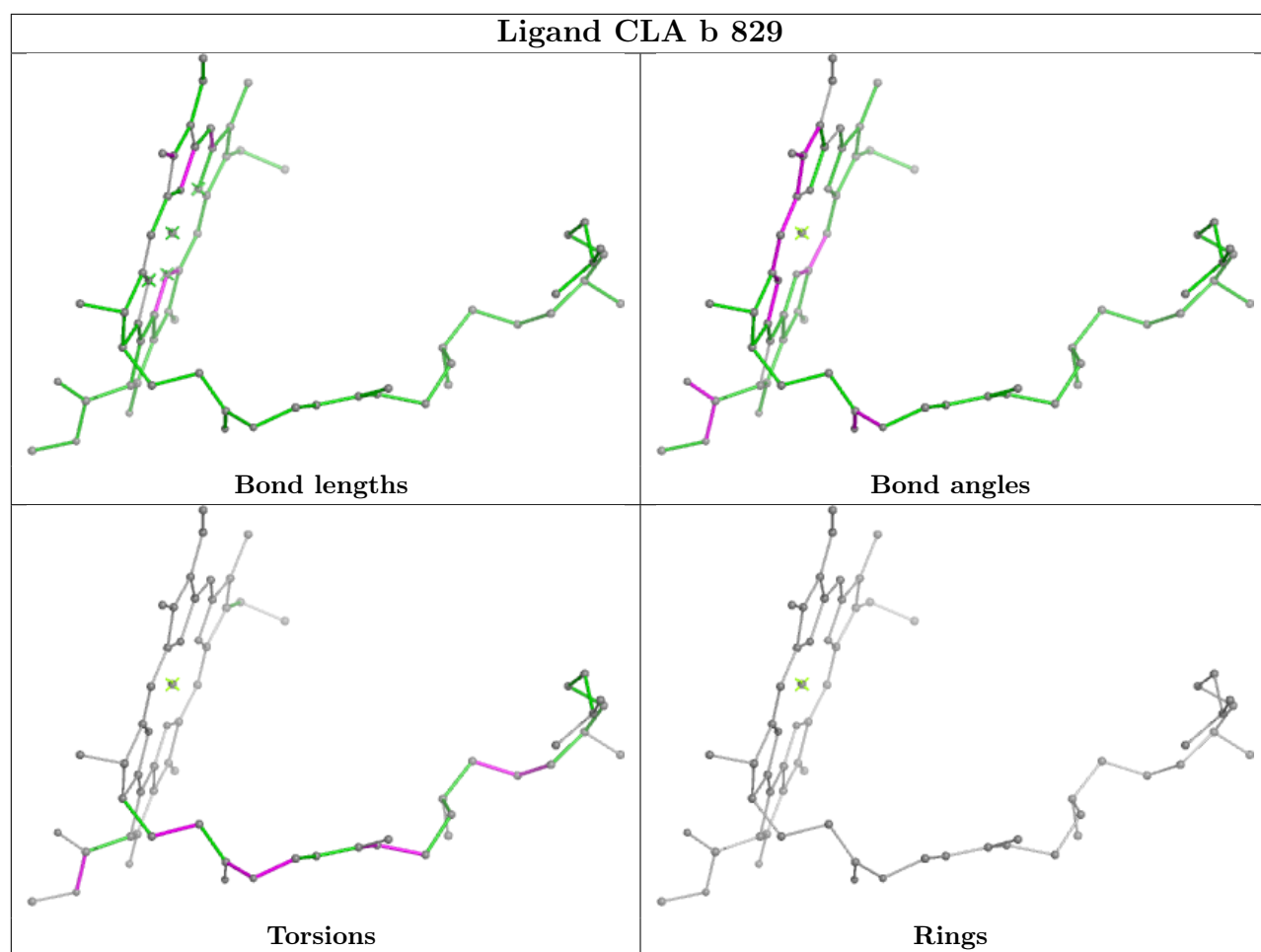




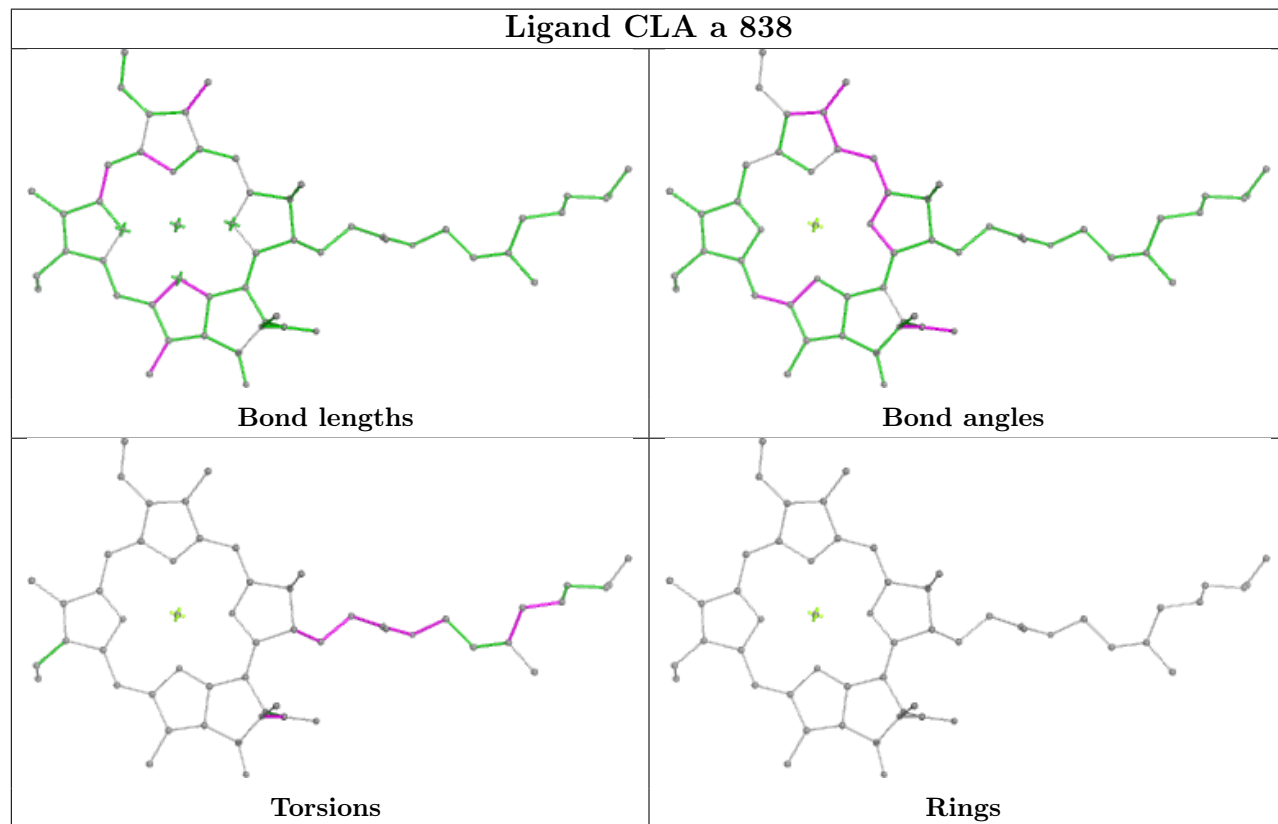
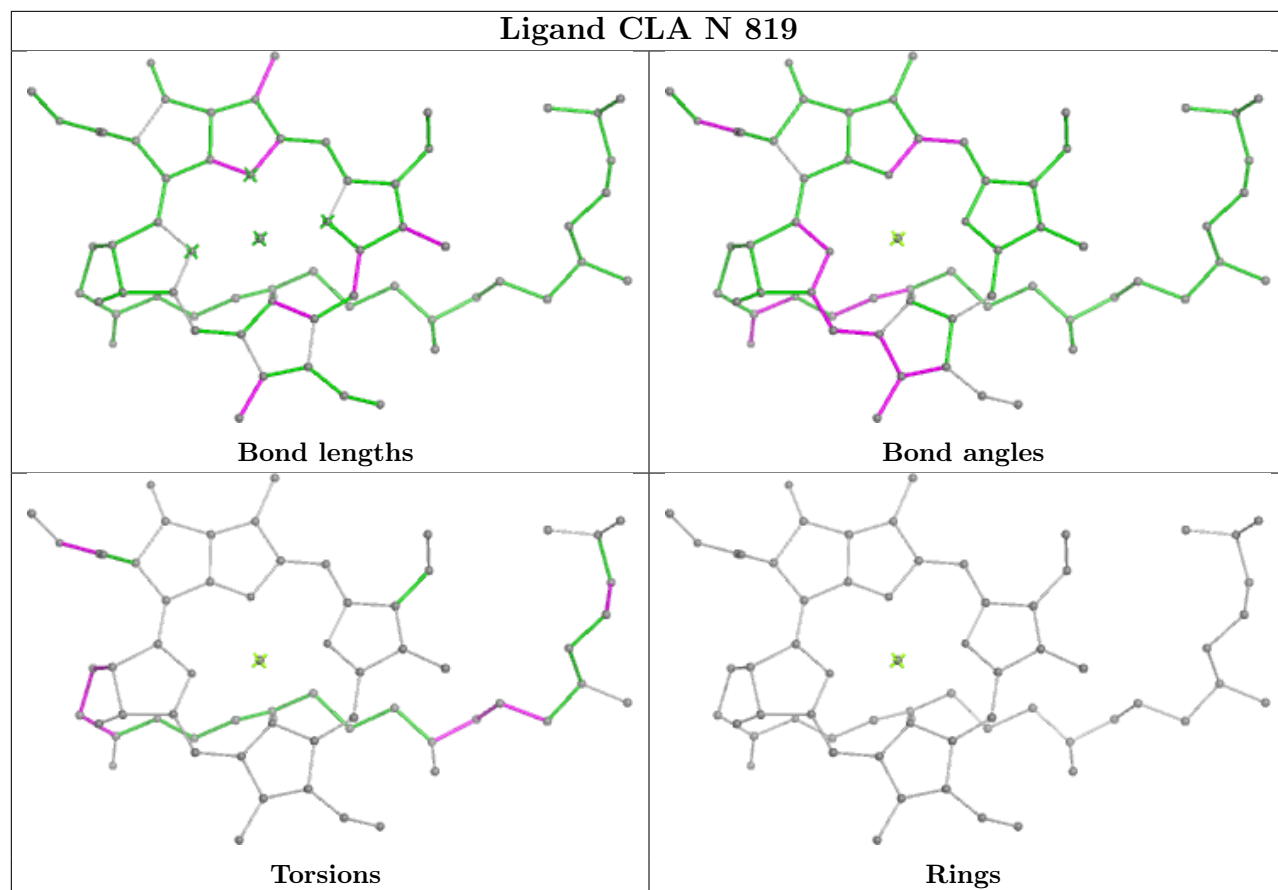




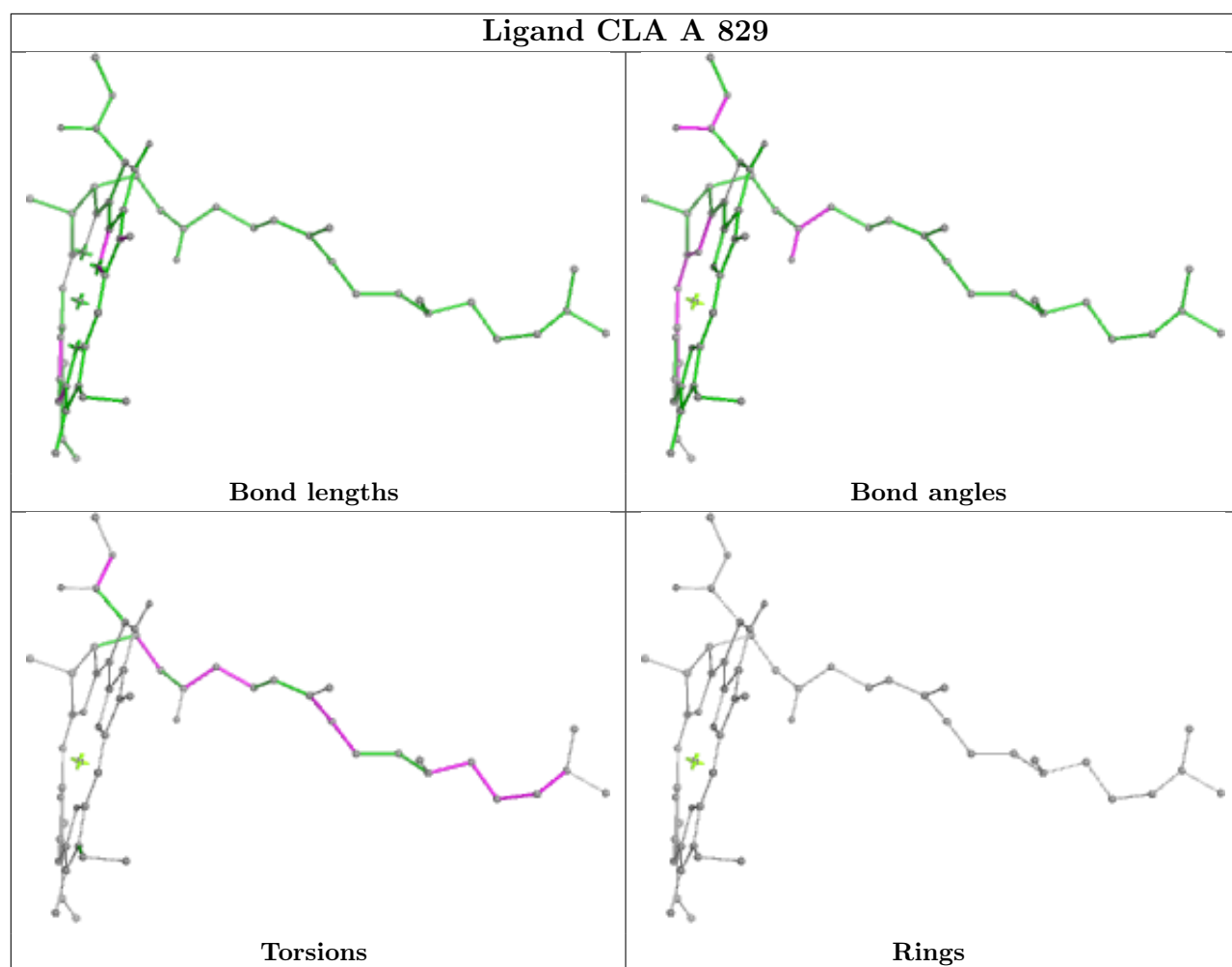






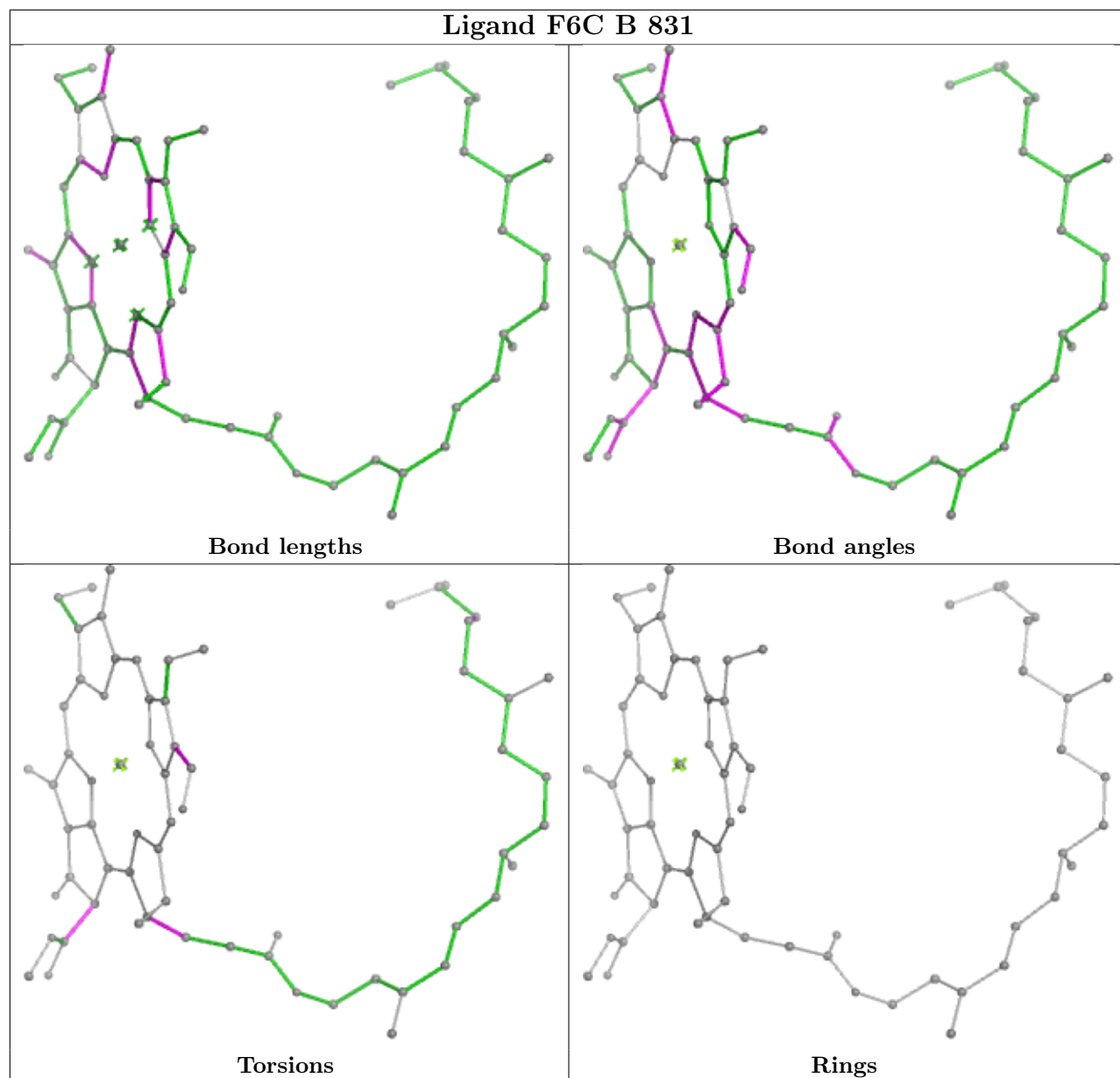






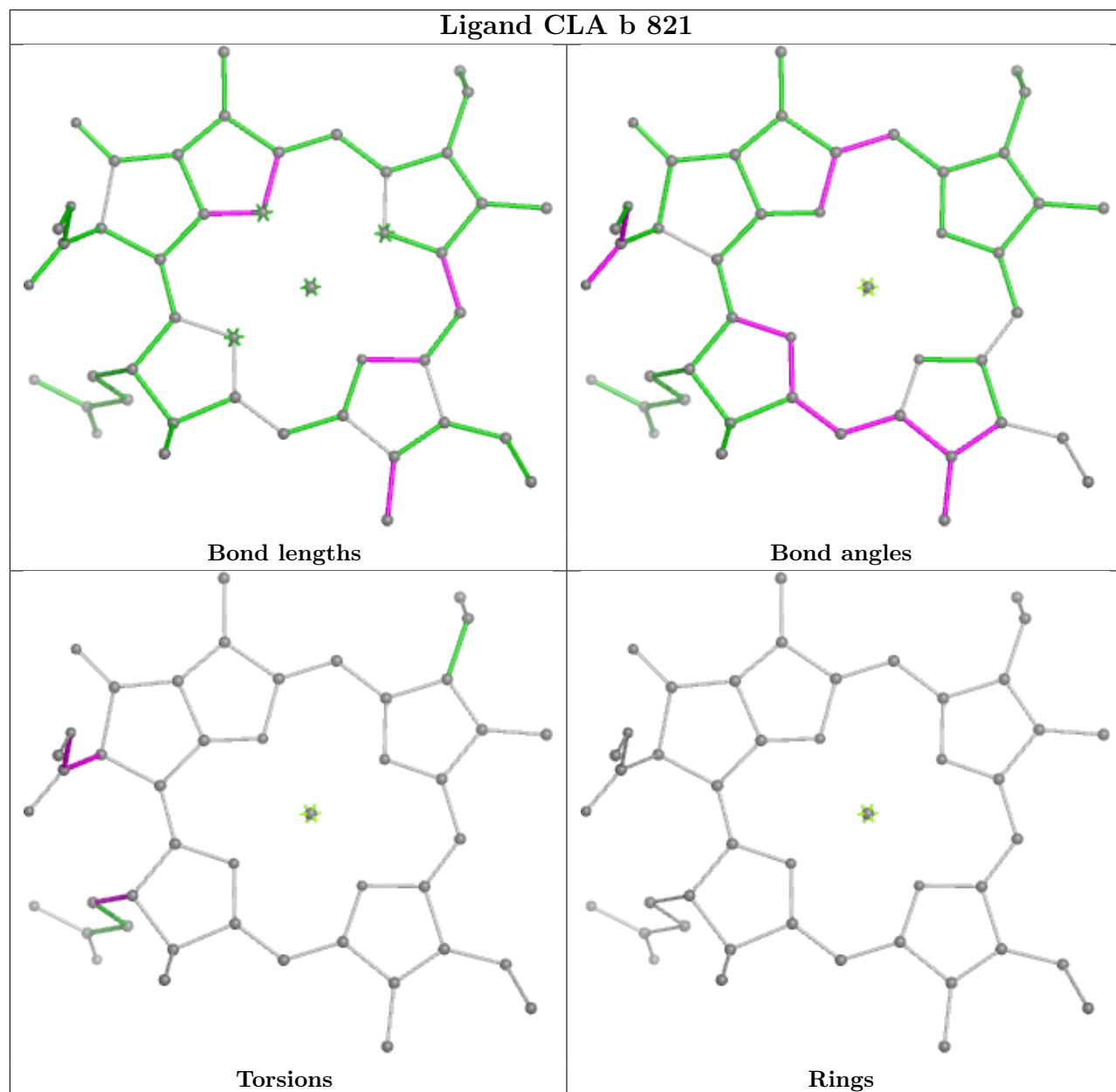


## Ligand F6C B 831

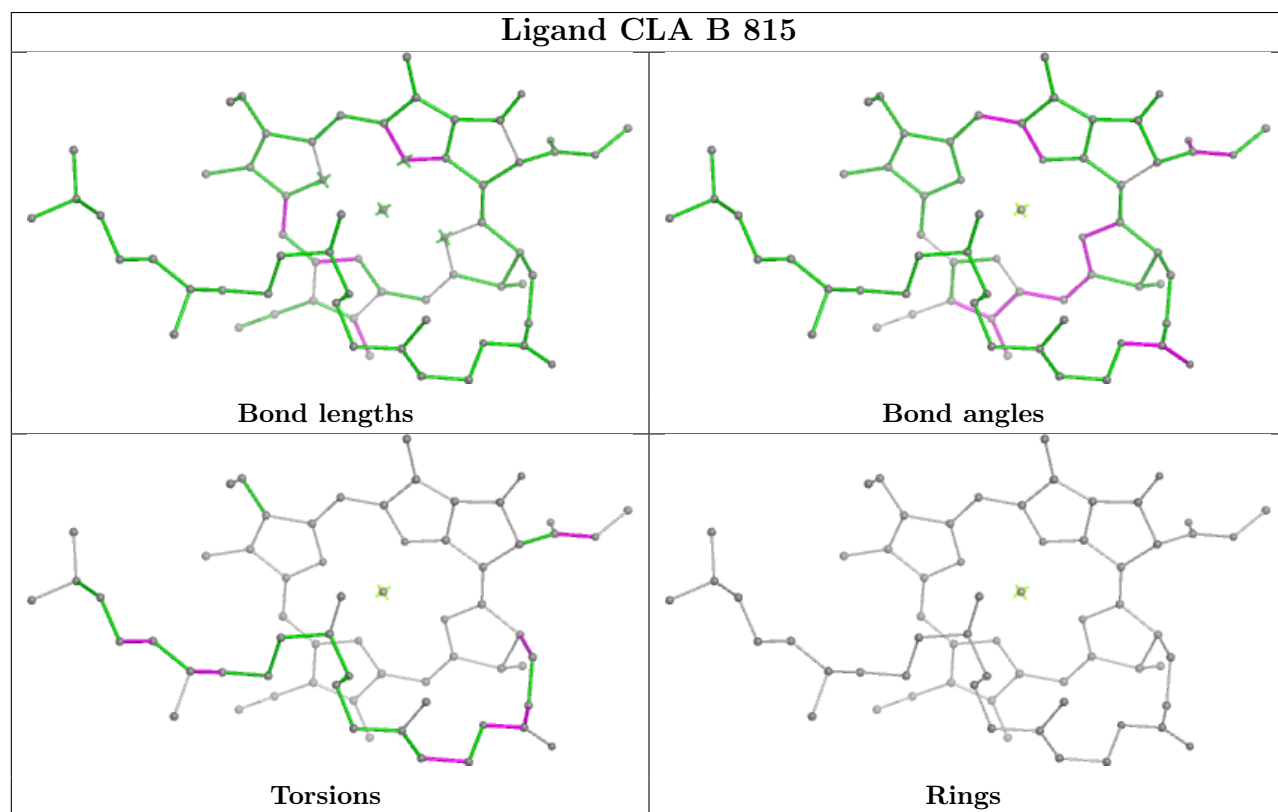
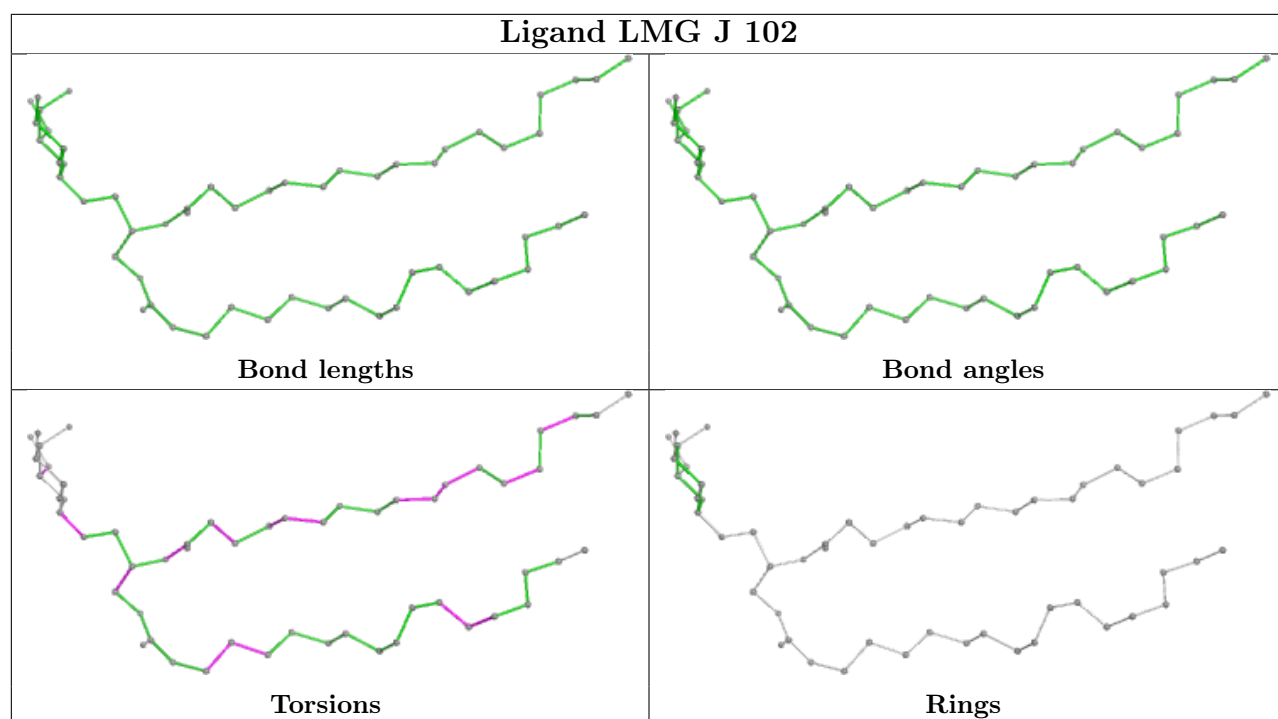




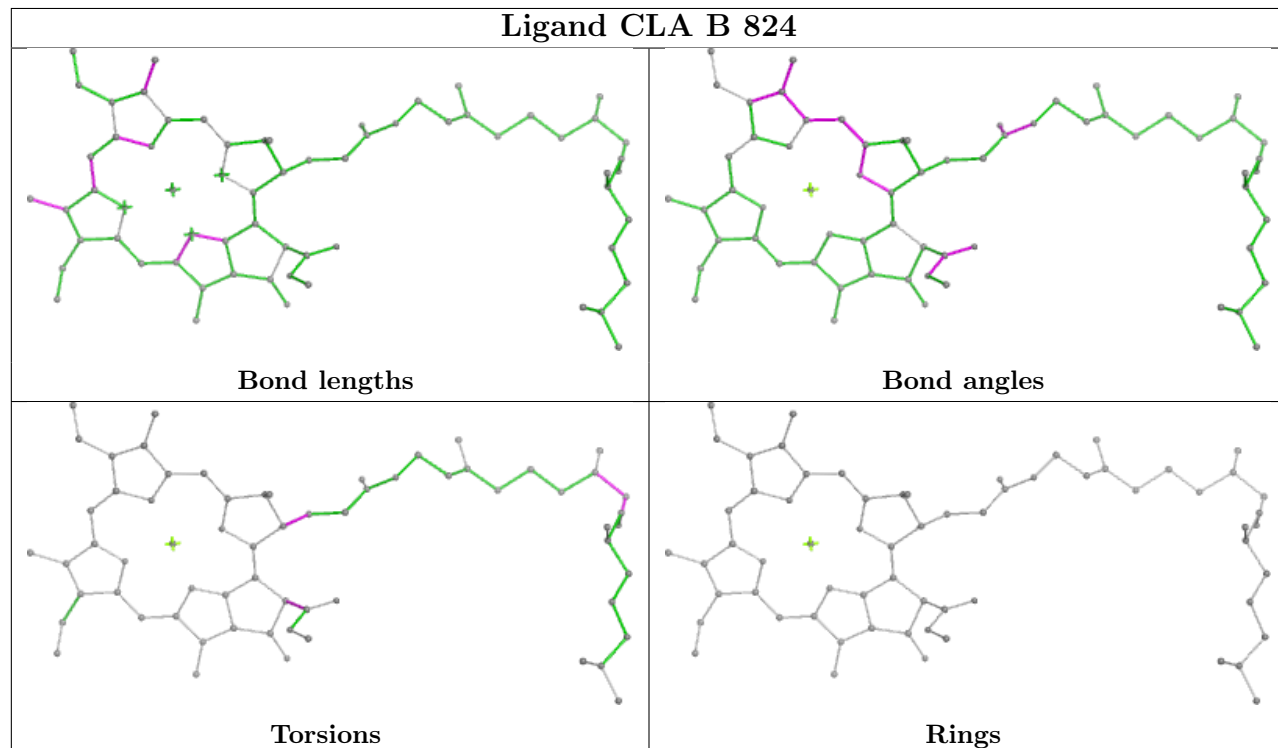
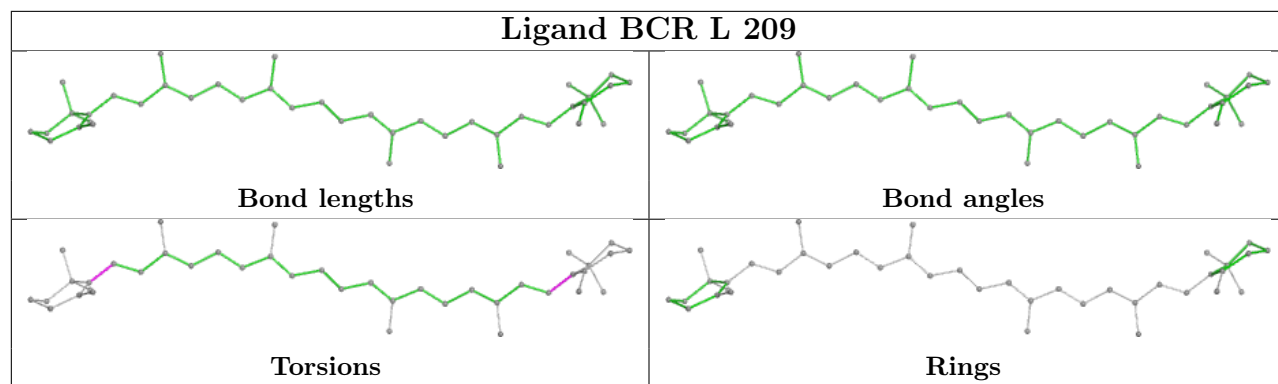
## Ligand CLA b 821



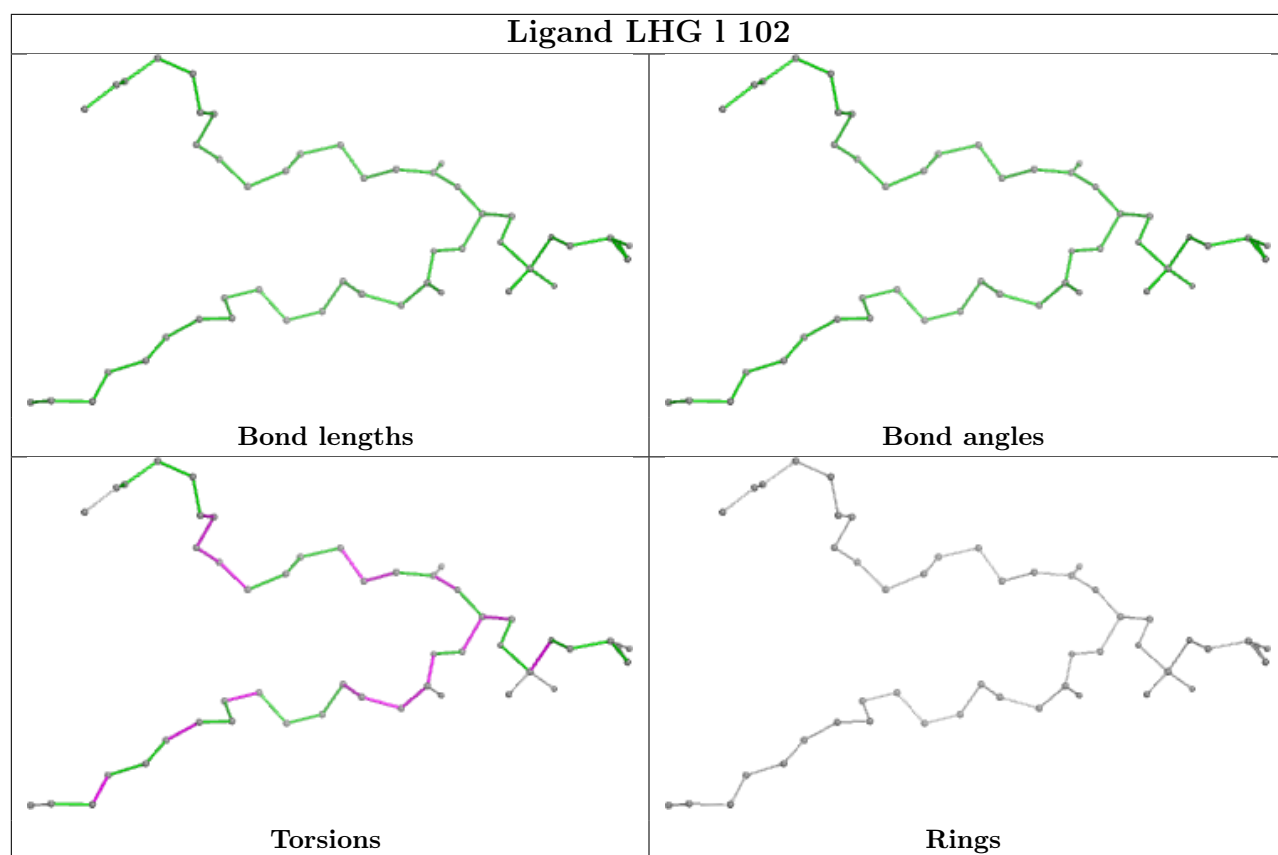






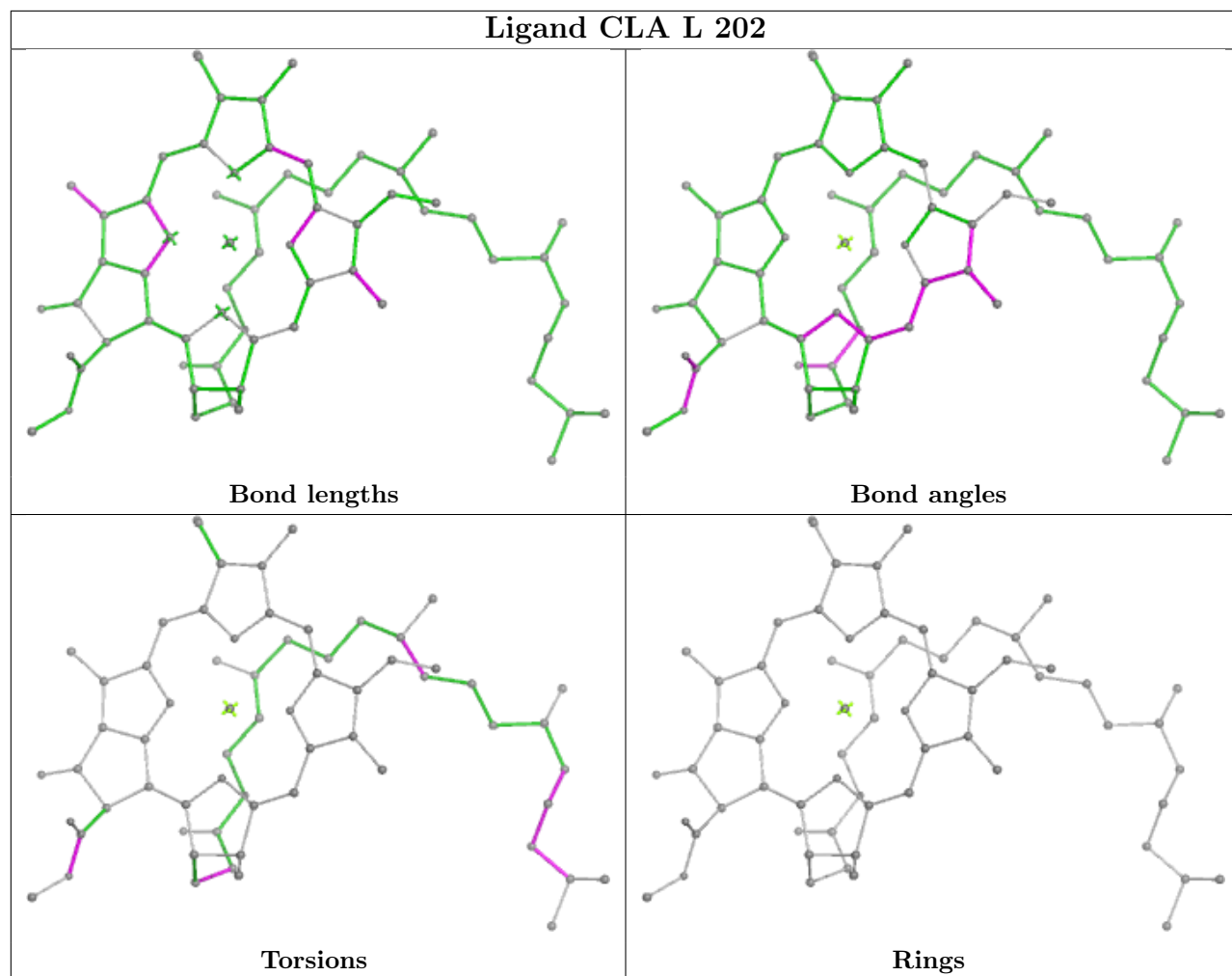




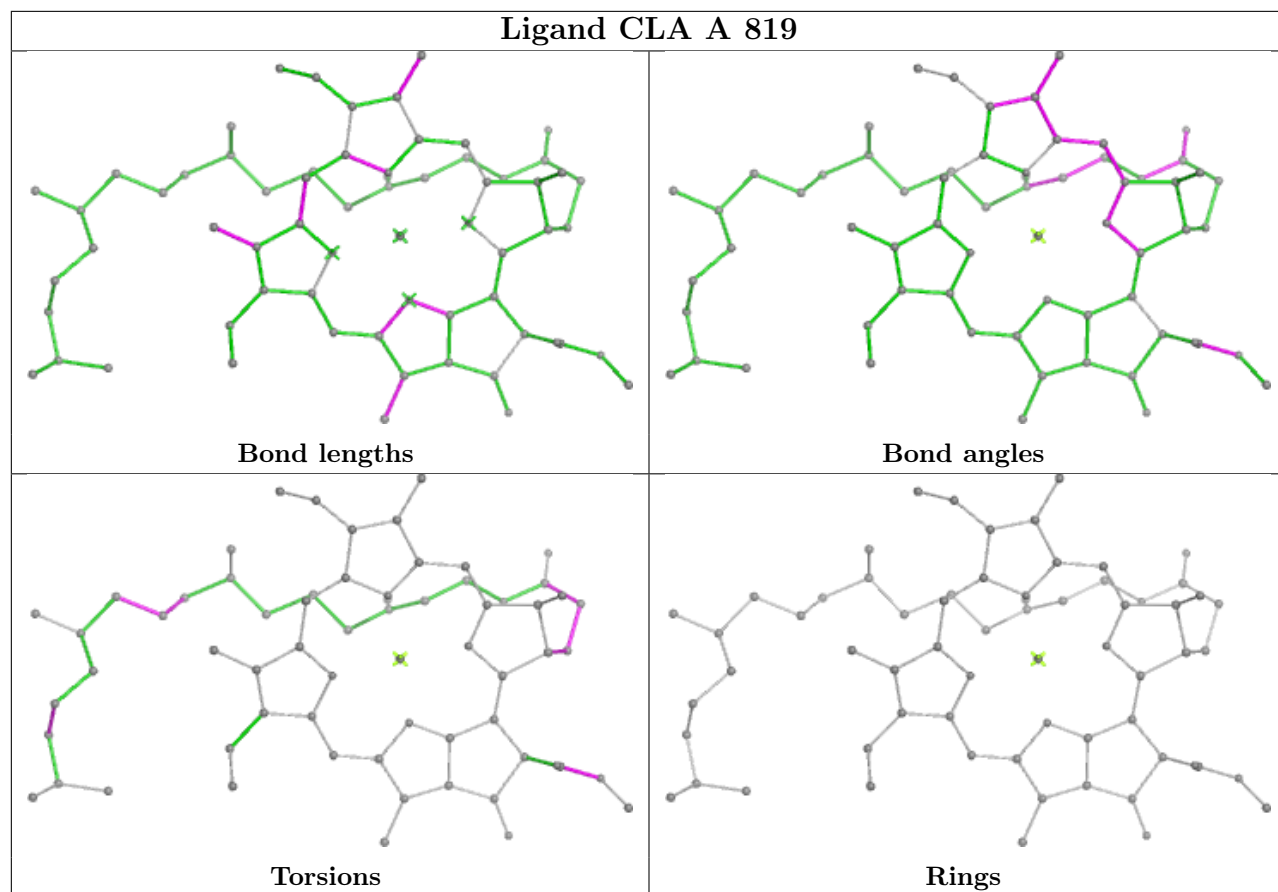




## Ligand CLA L 202

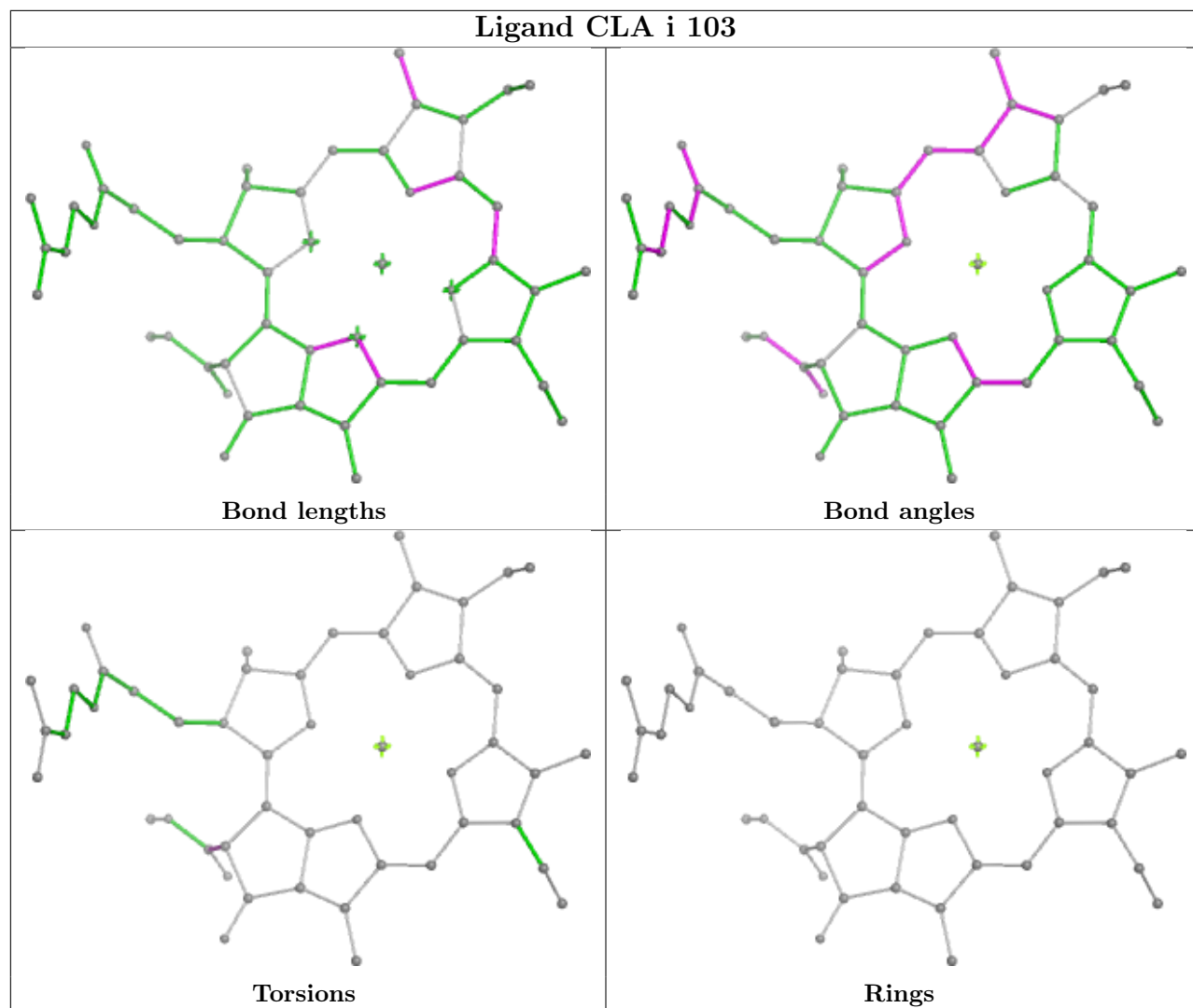






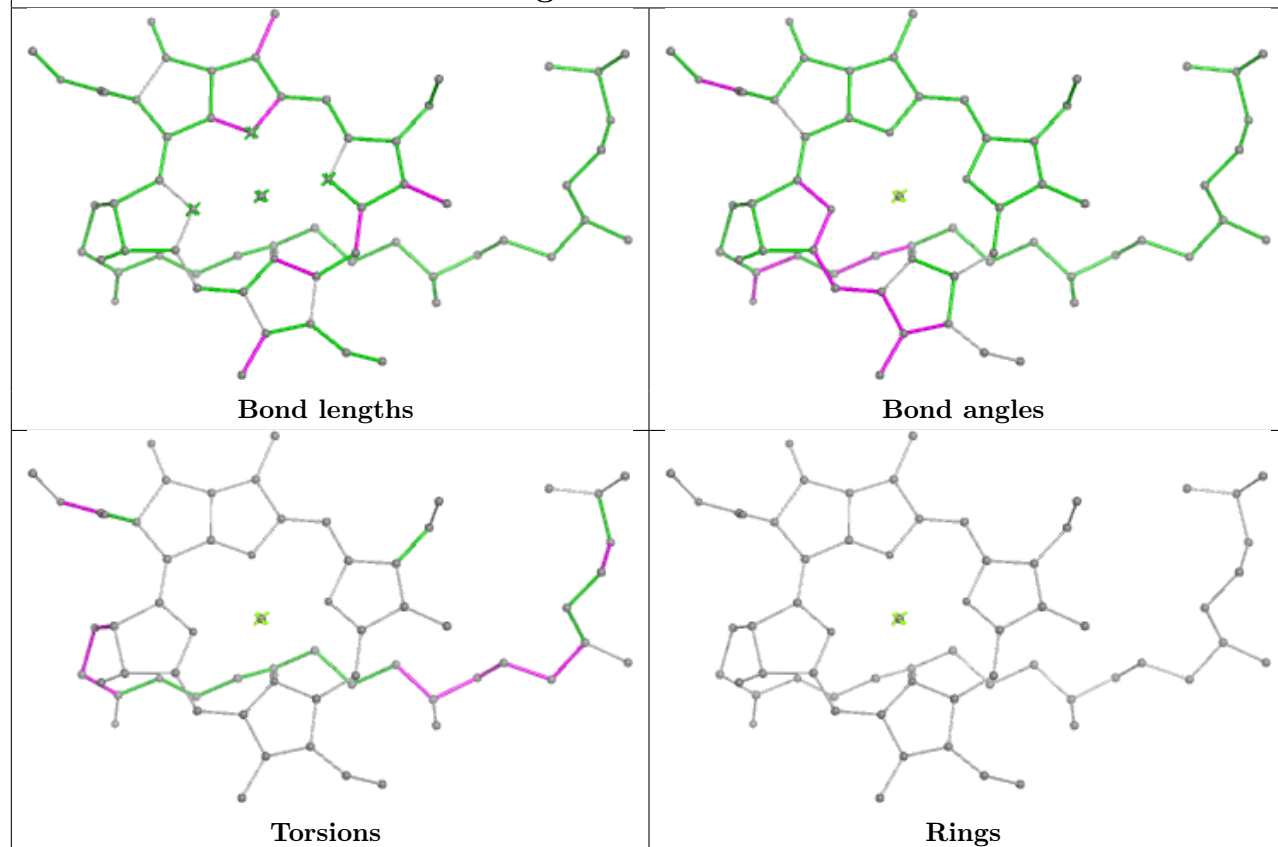


## Ligand CLA i 103

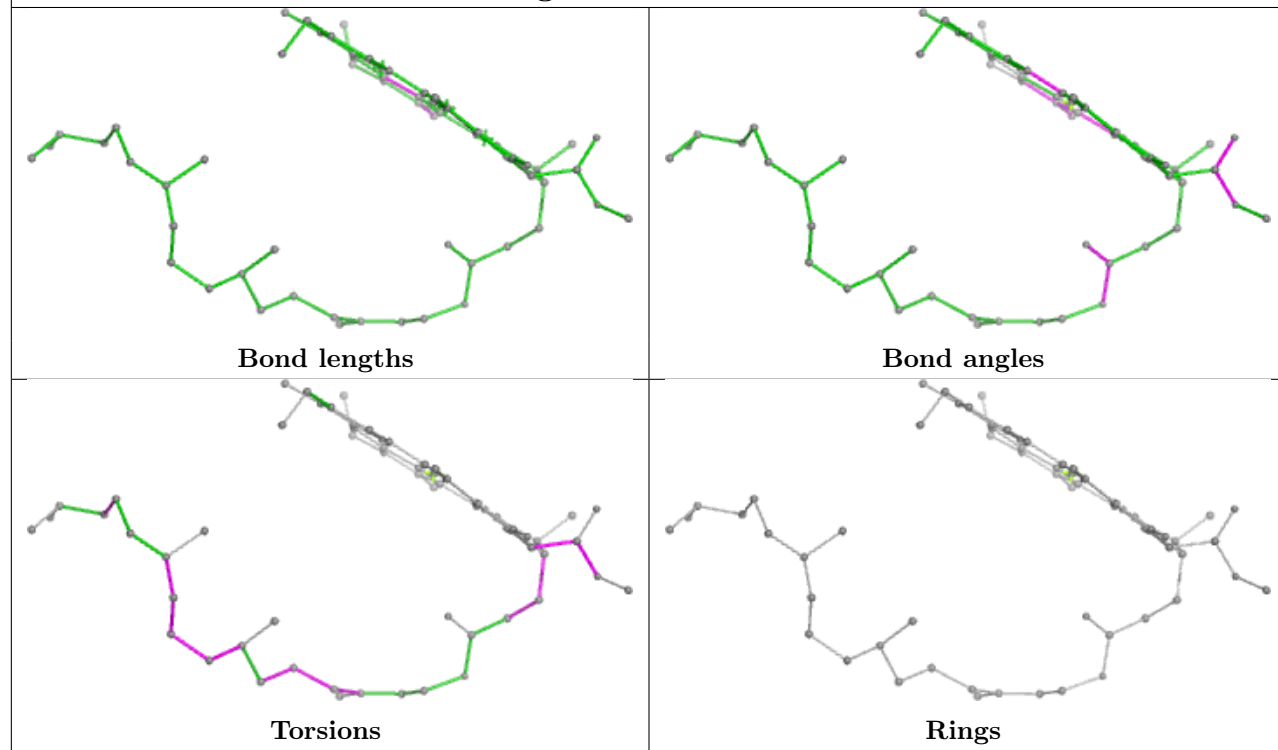




## Ligand CLA a 819

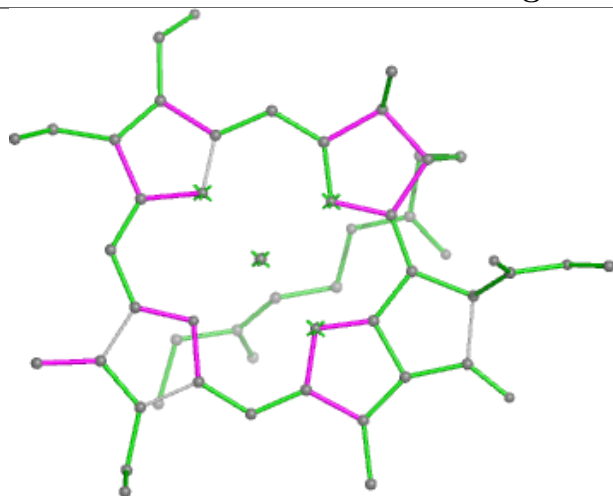


## Ligand CLA a 812

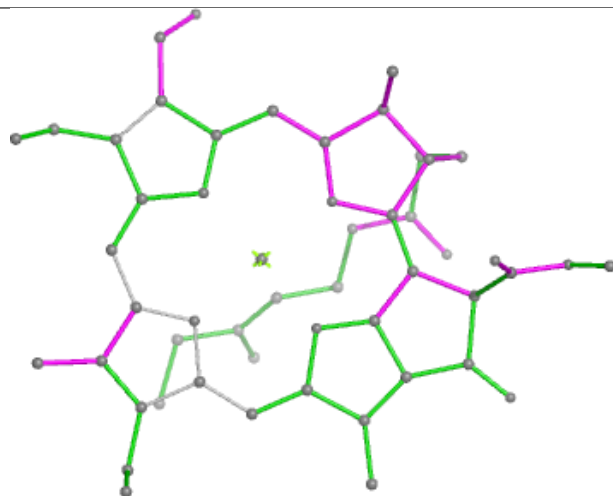




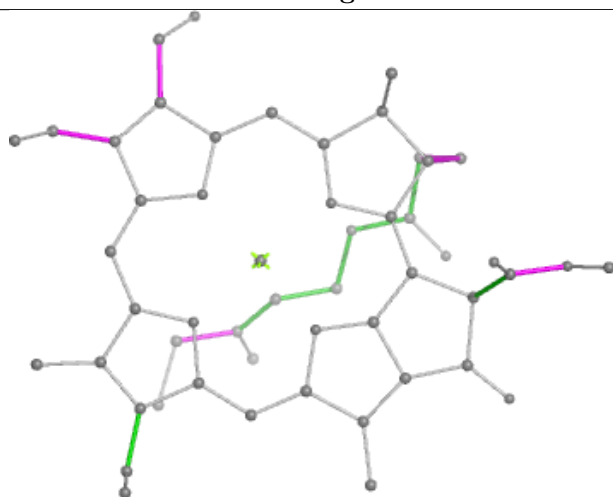
## Ligand F6C a 824



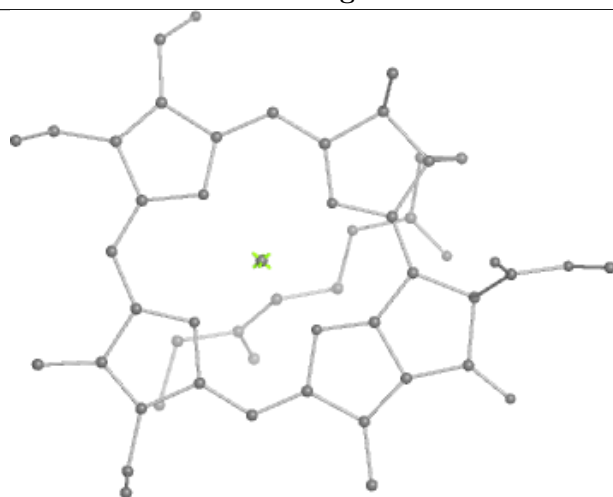
Bond lengths



Bond angles

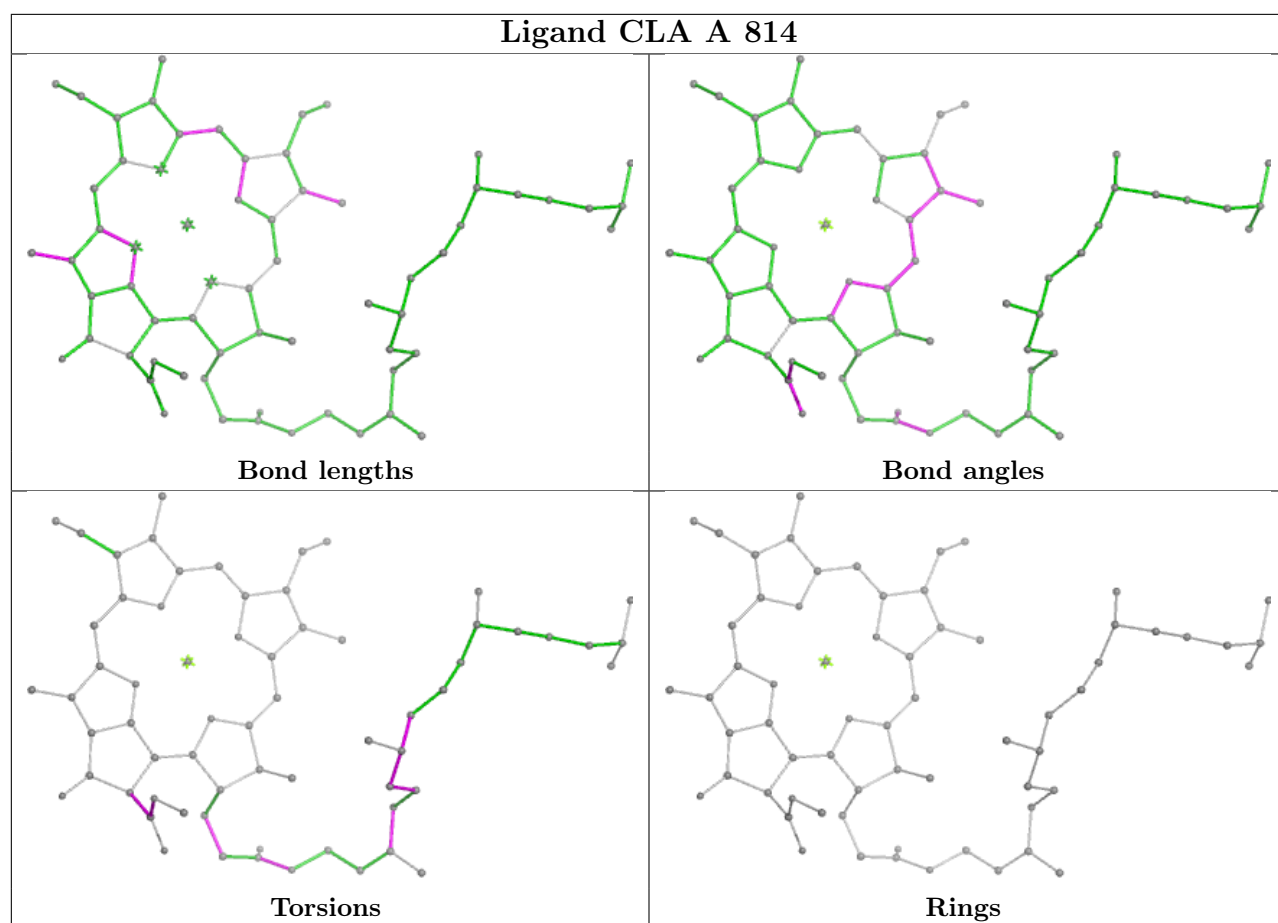


Torsions



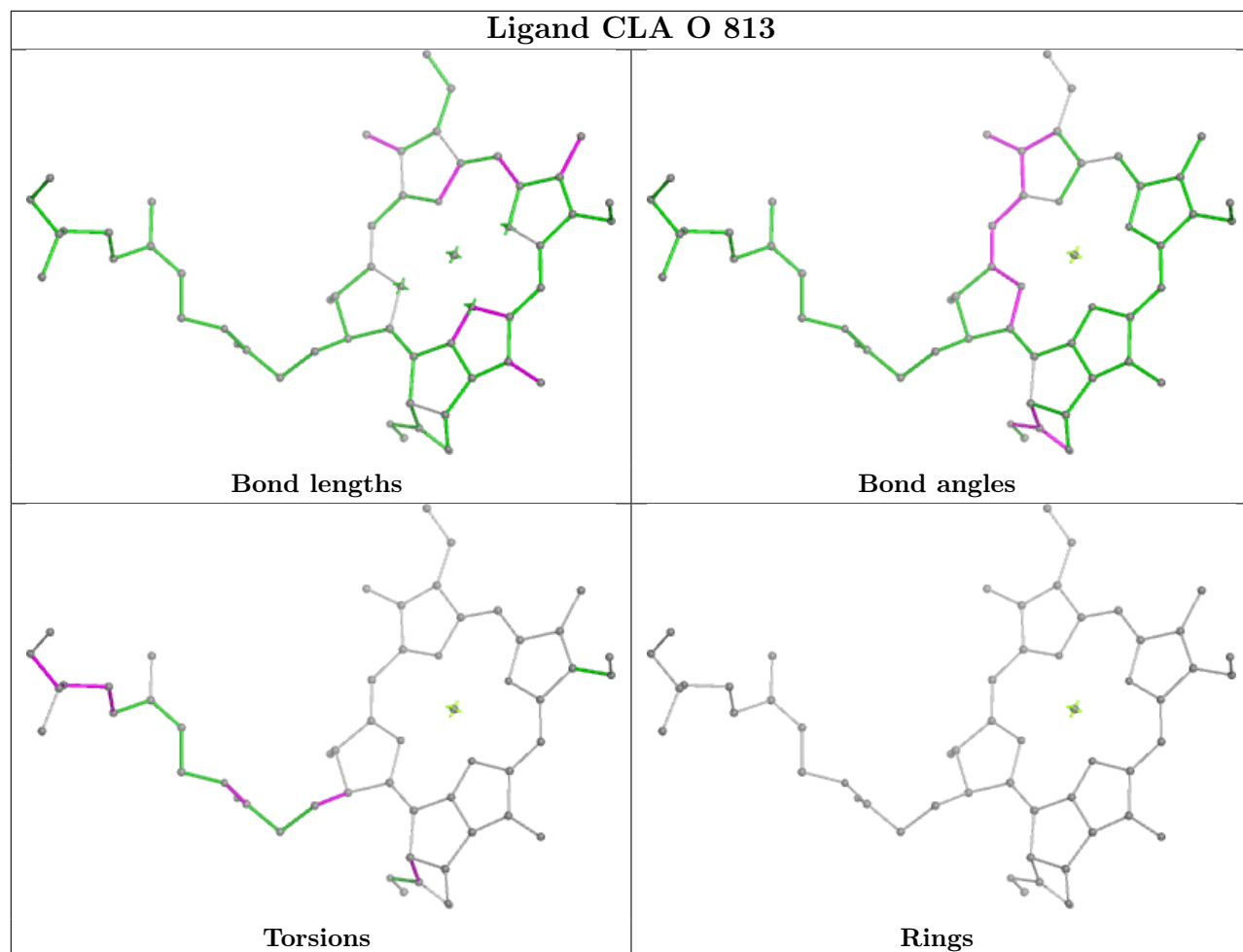
Rings



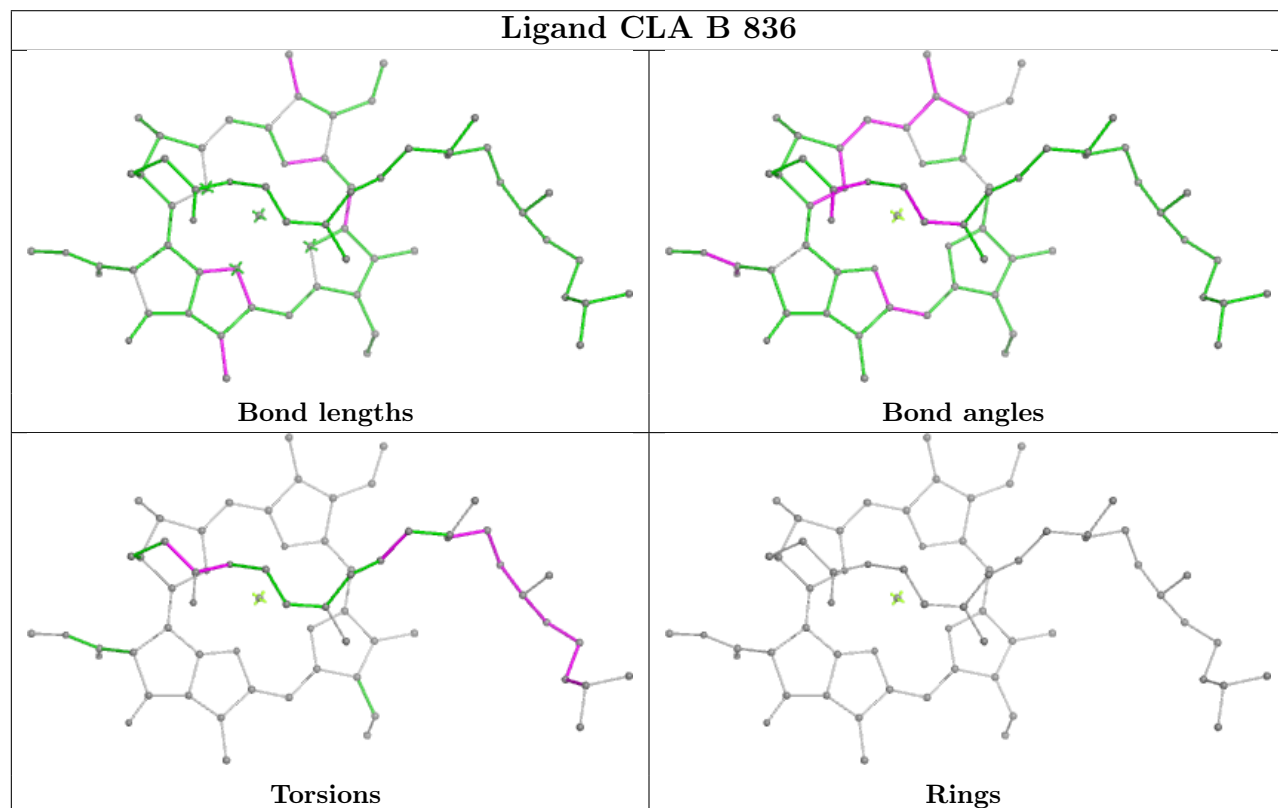




## Ligand CLA O 813

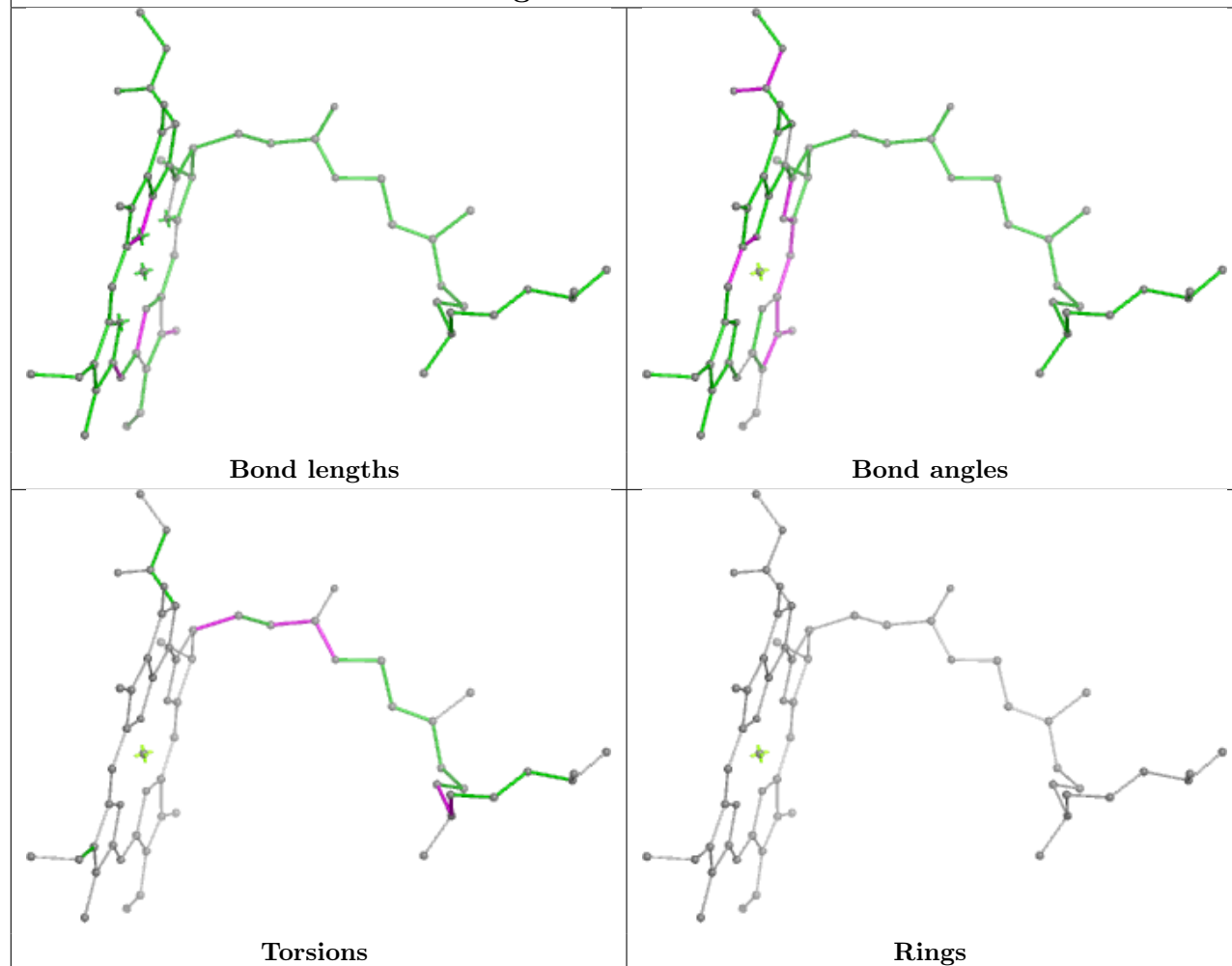


## Ligand CLA B 836

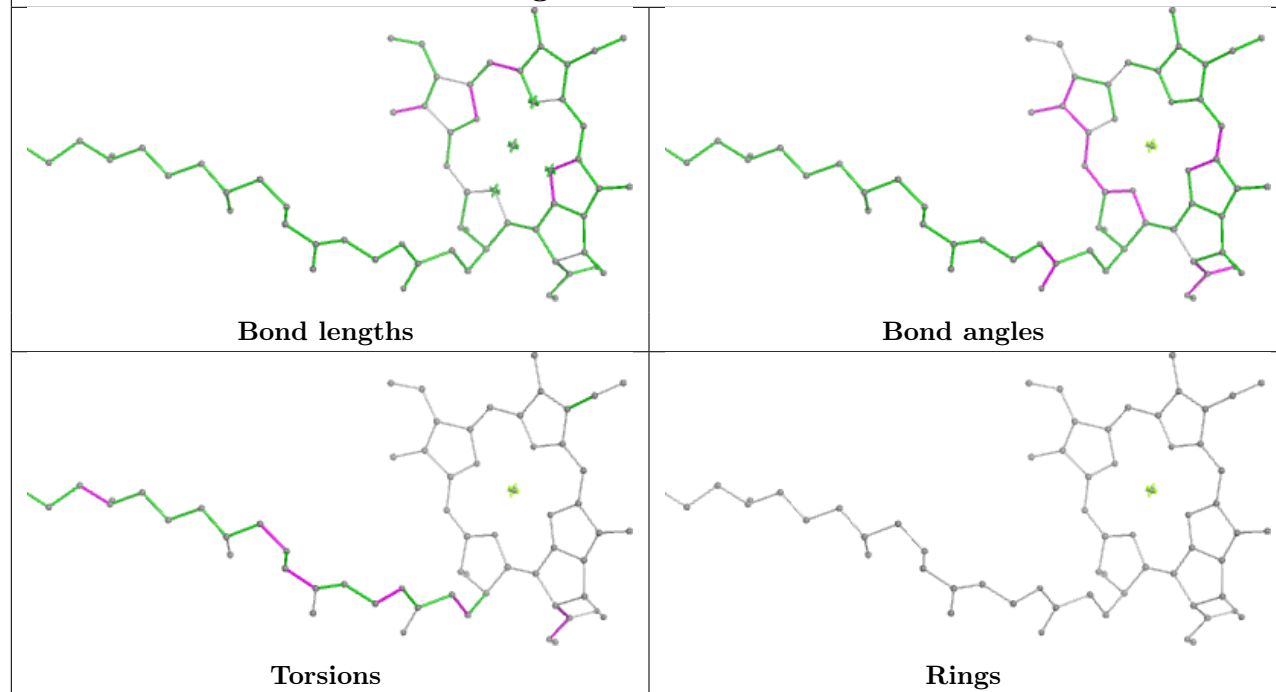




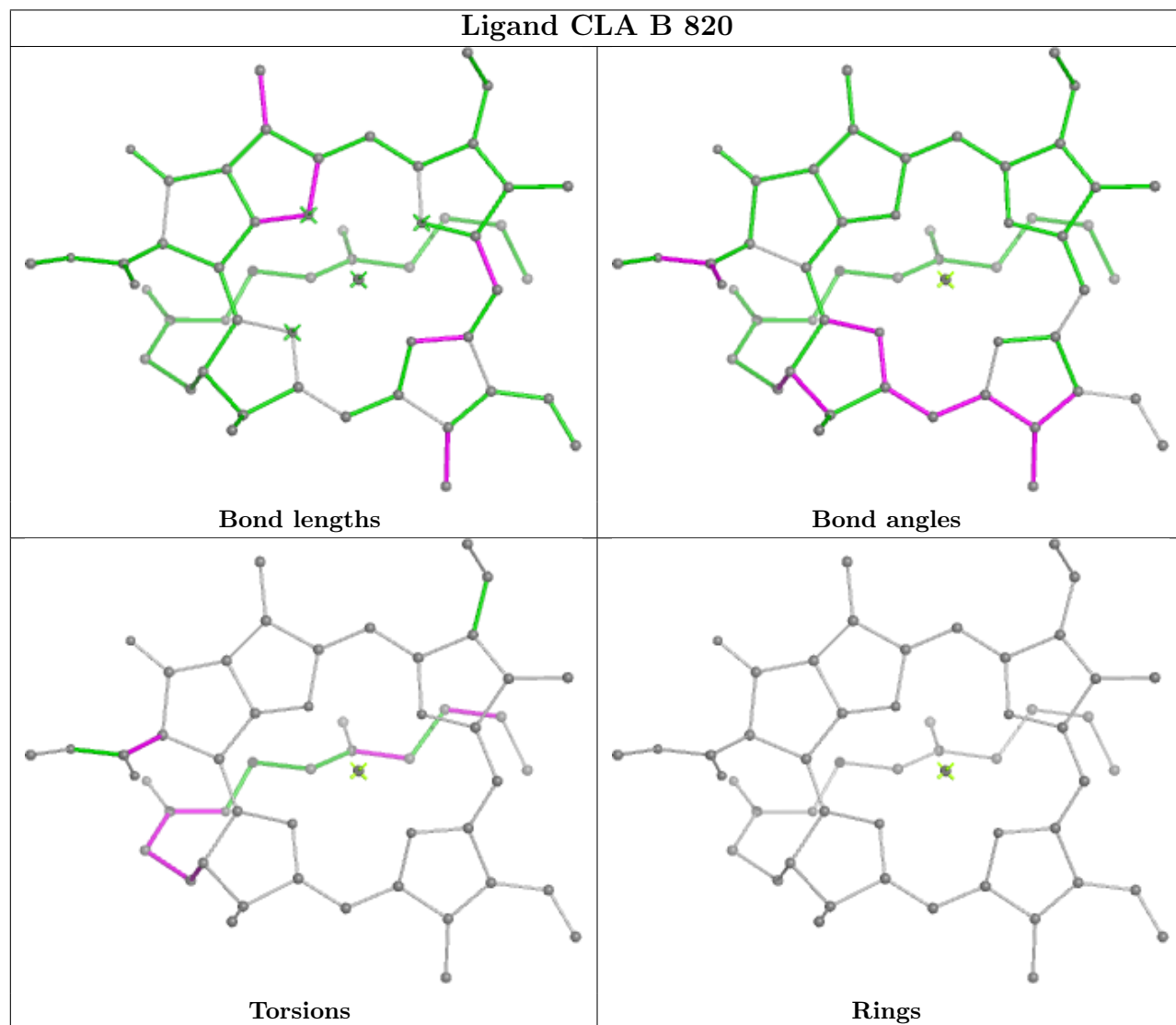
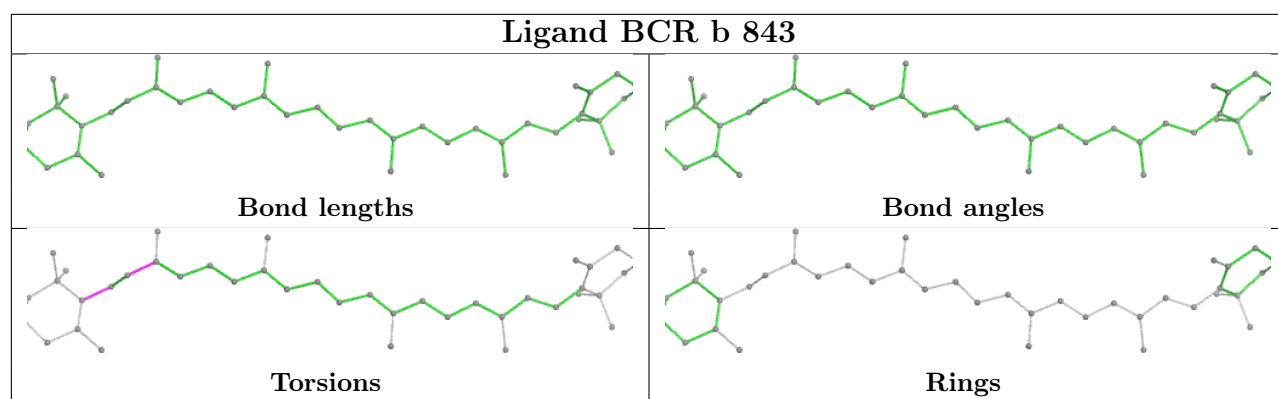
## Ligand CLA A 805



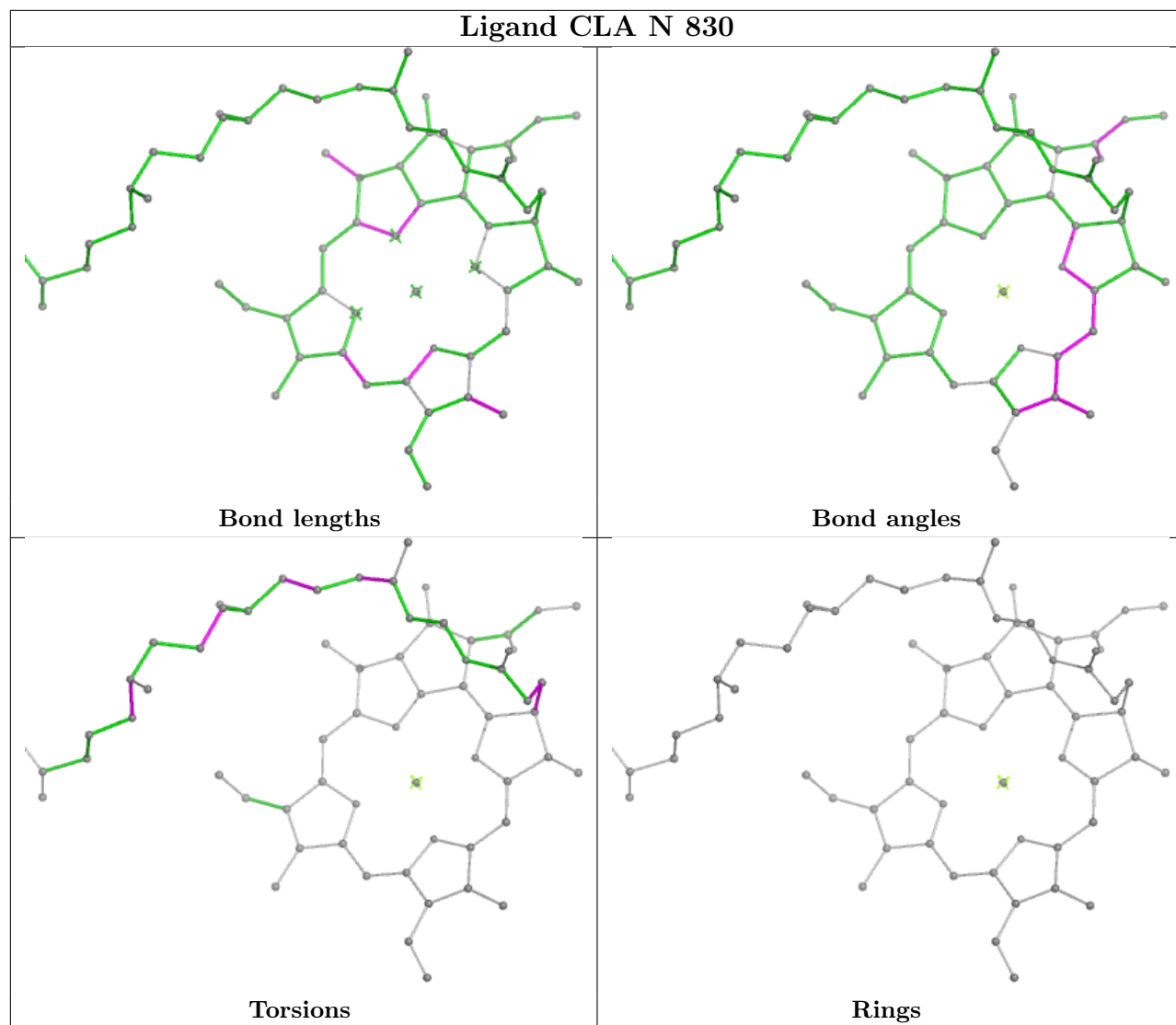
## Ligand CLA N 835



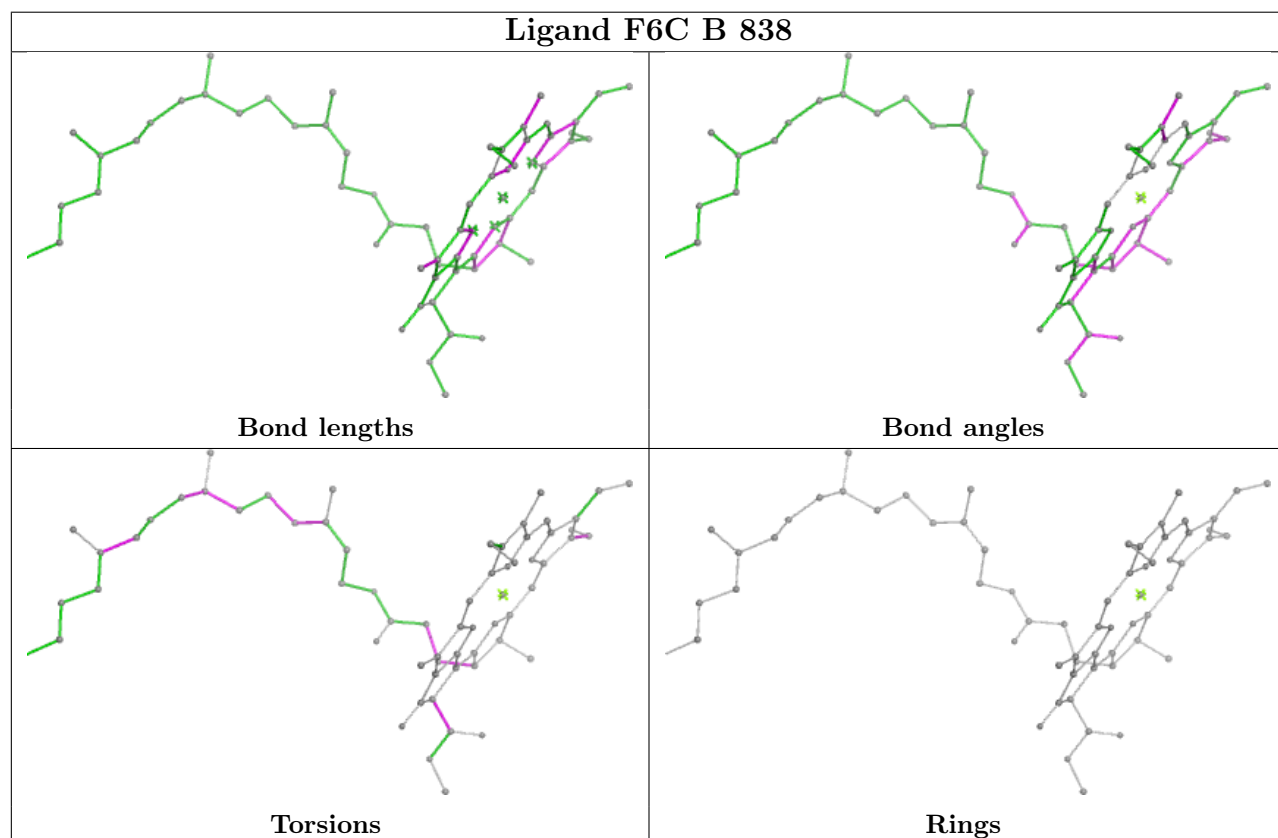
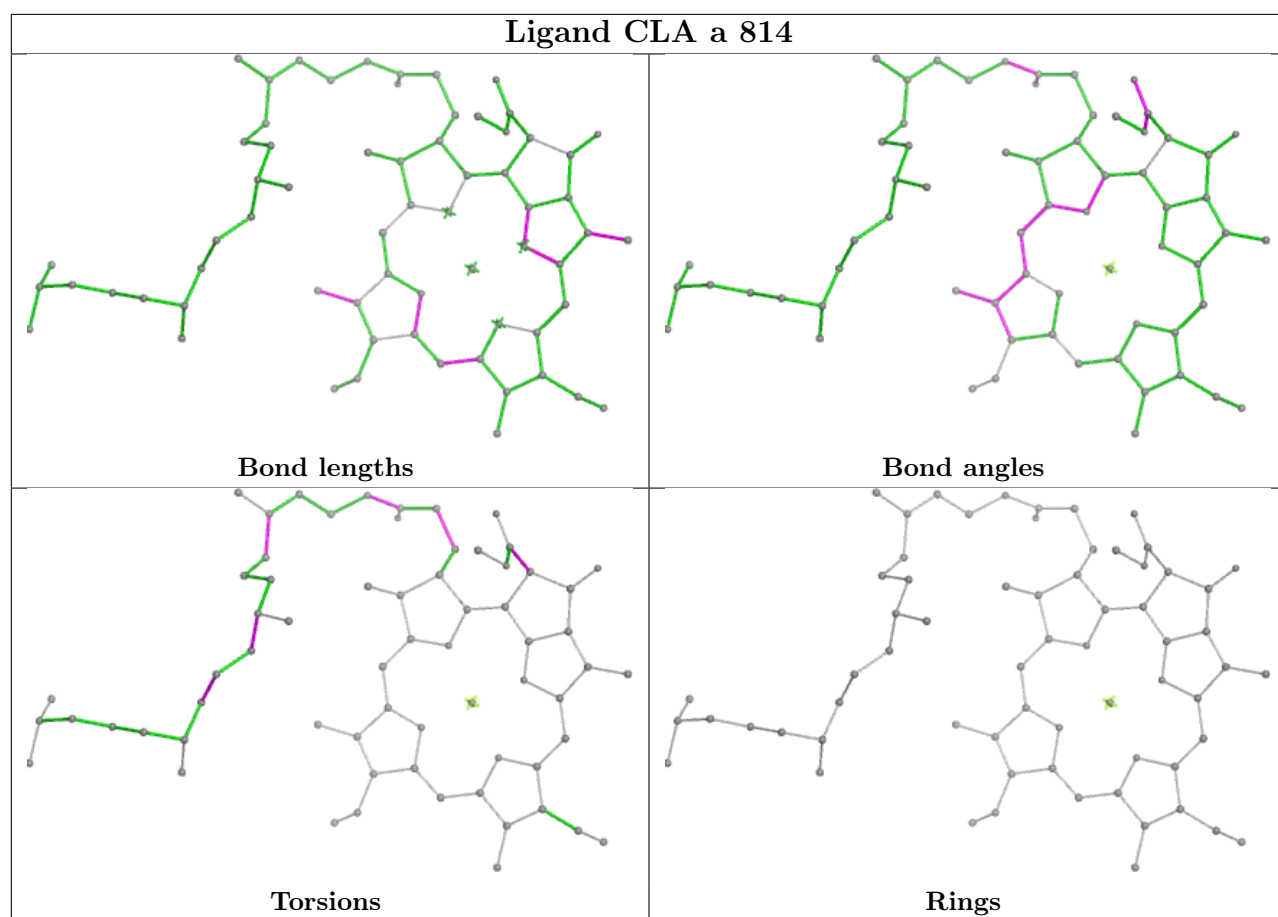




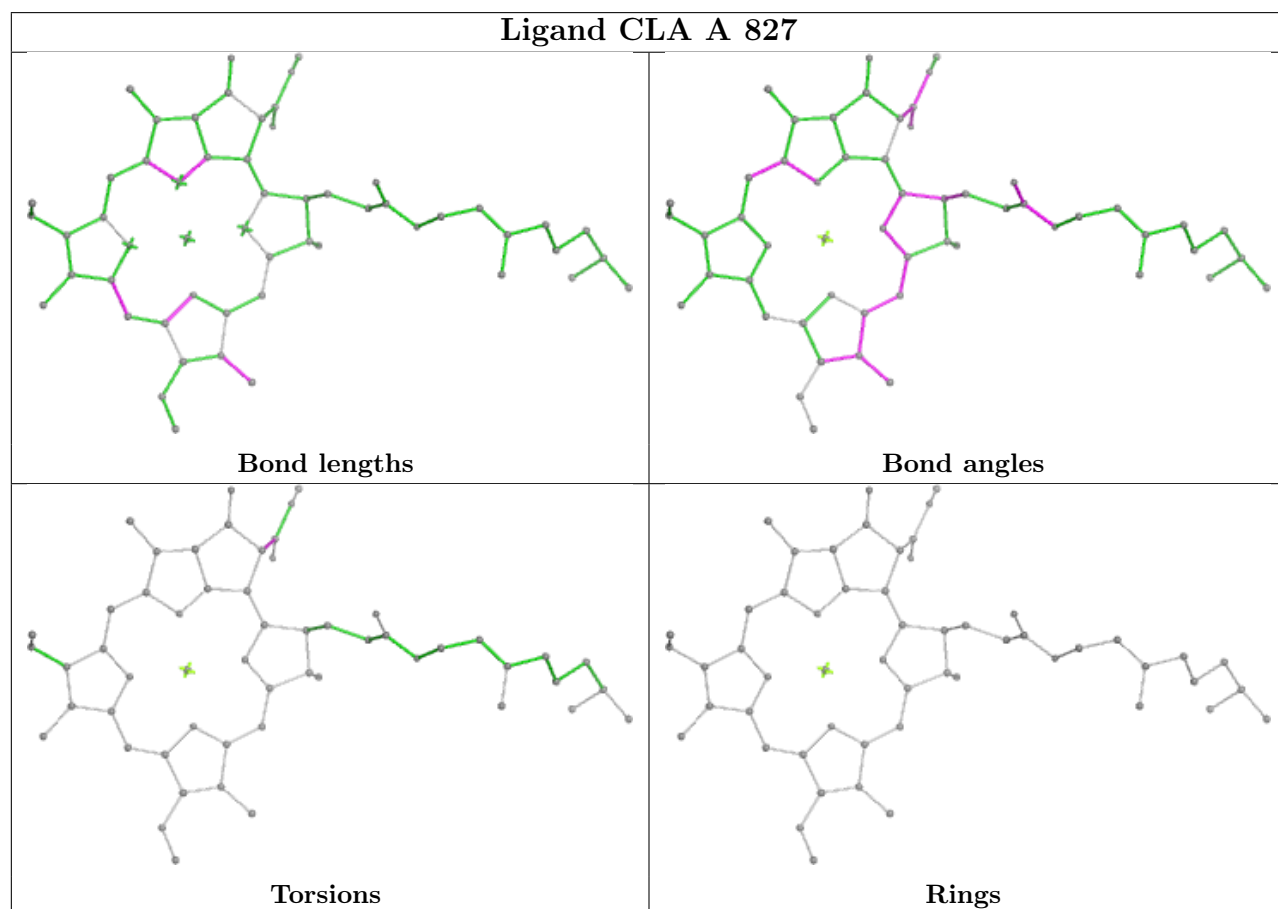
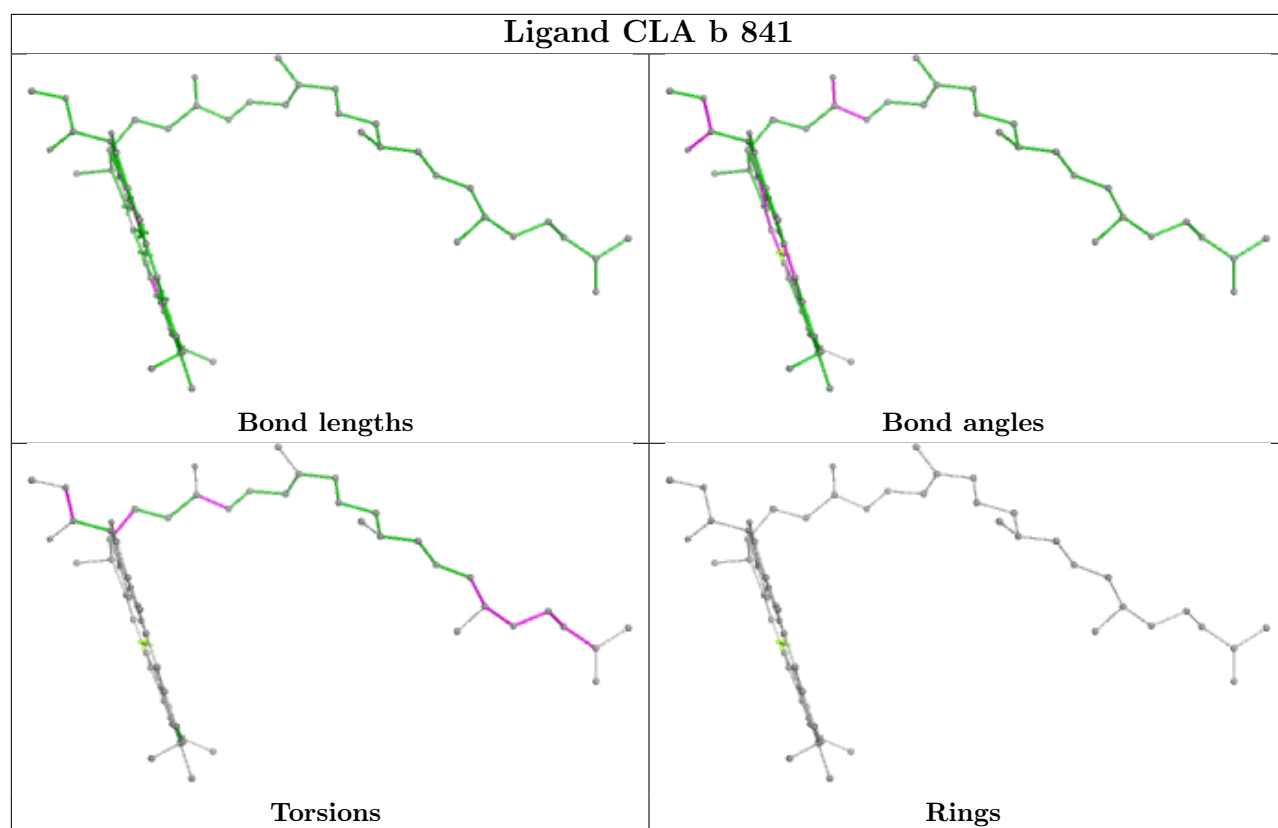




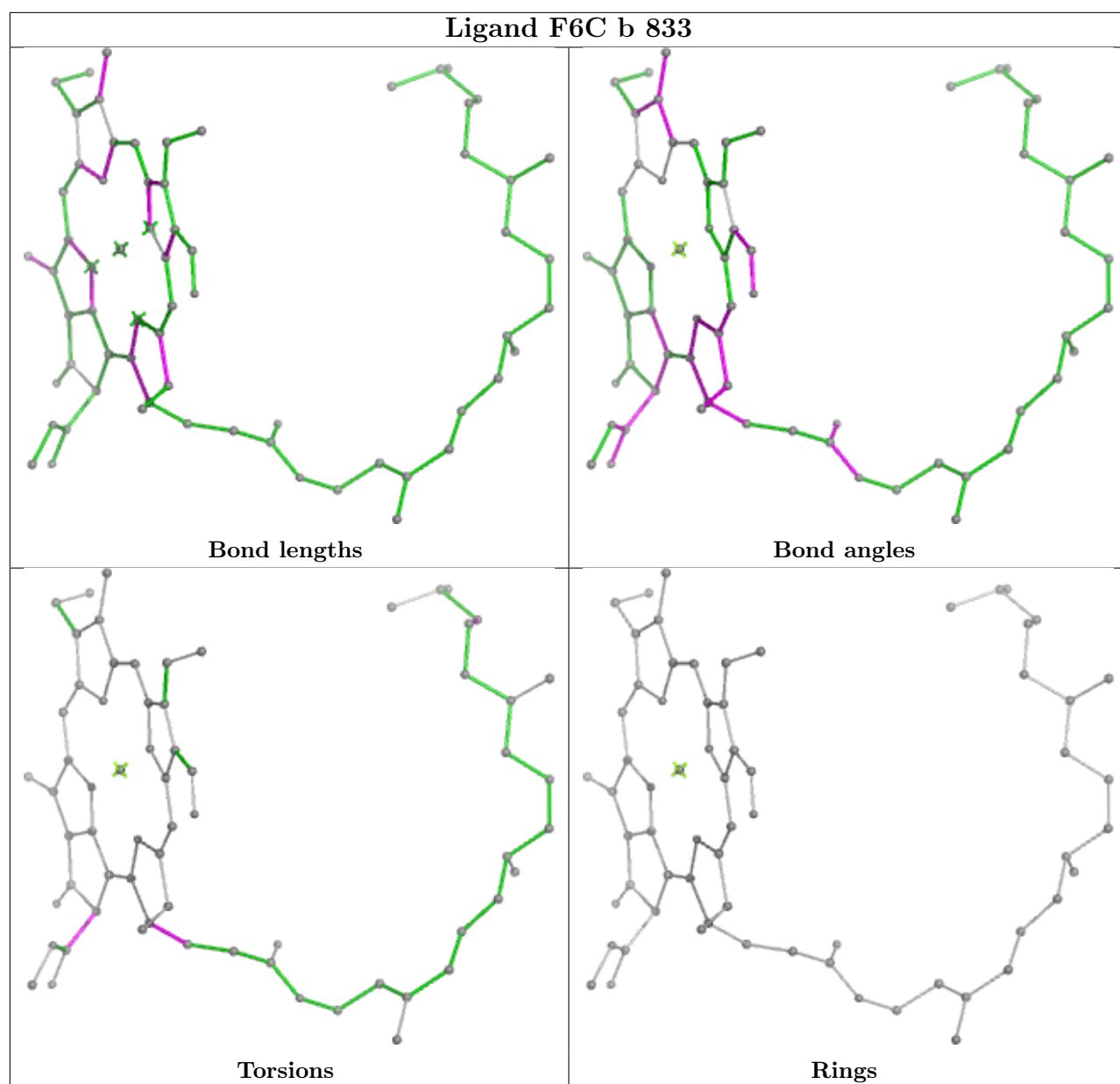




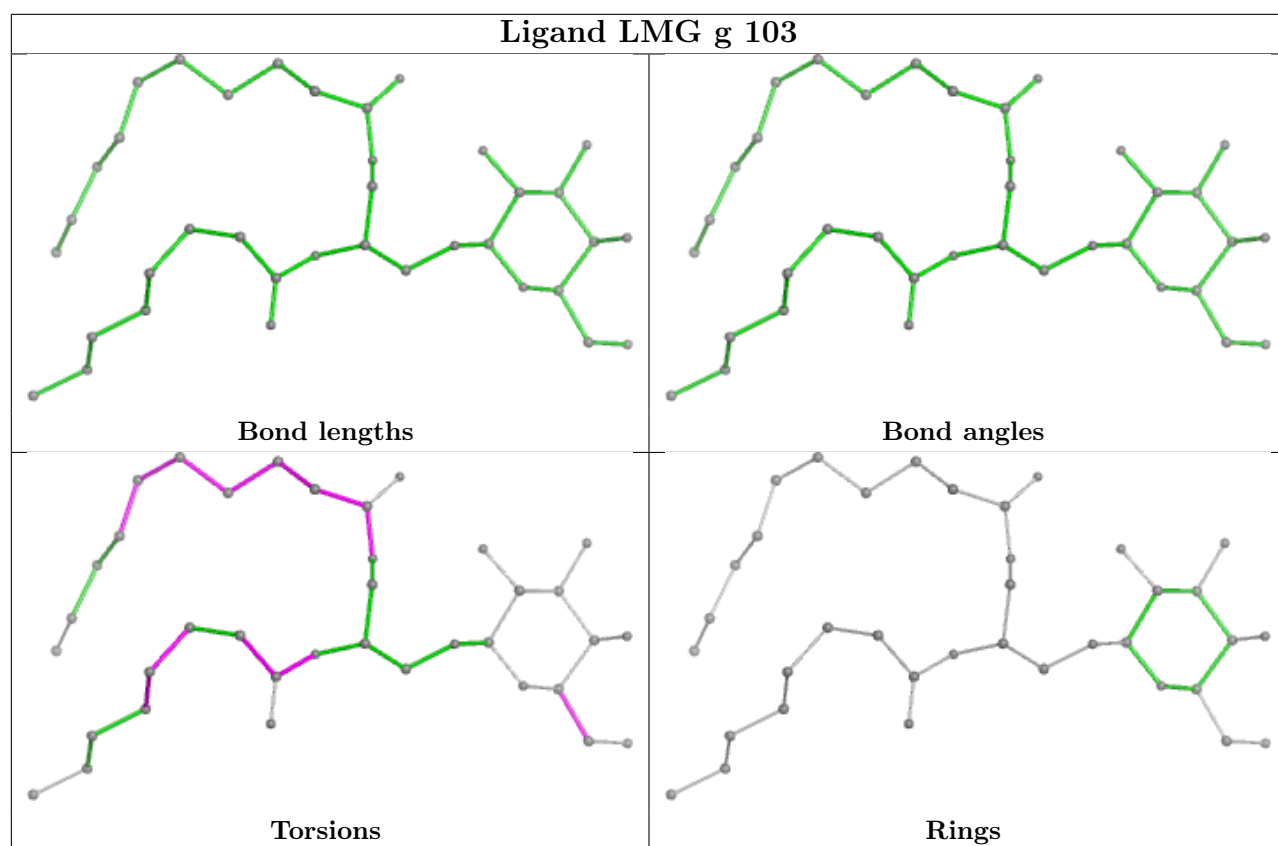






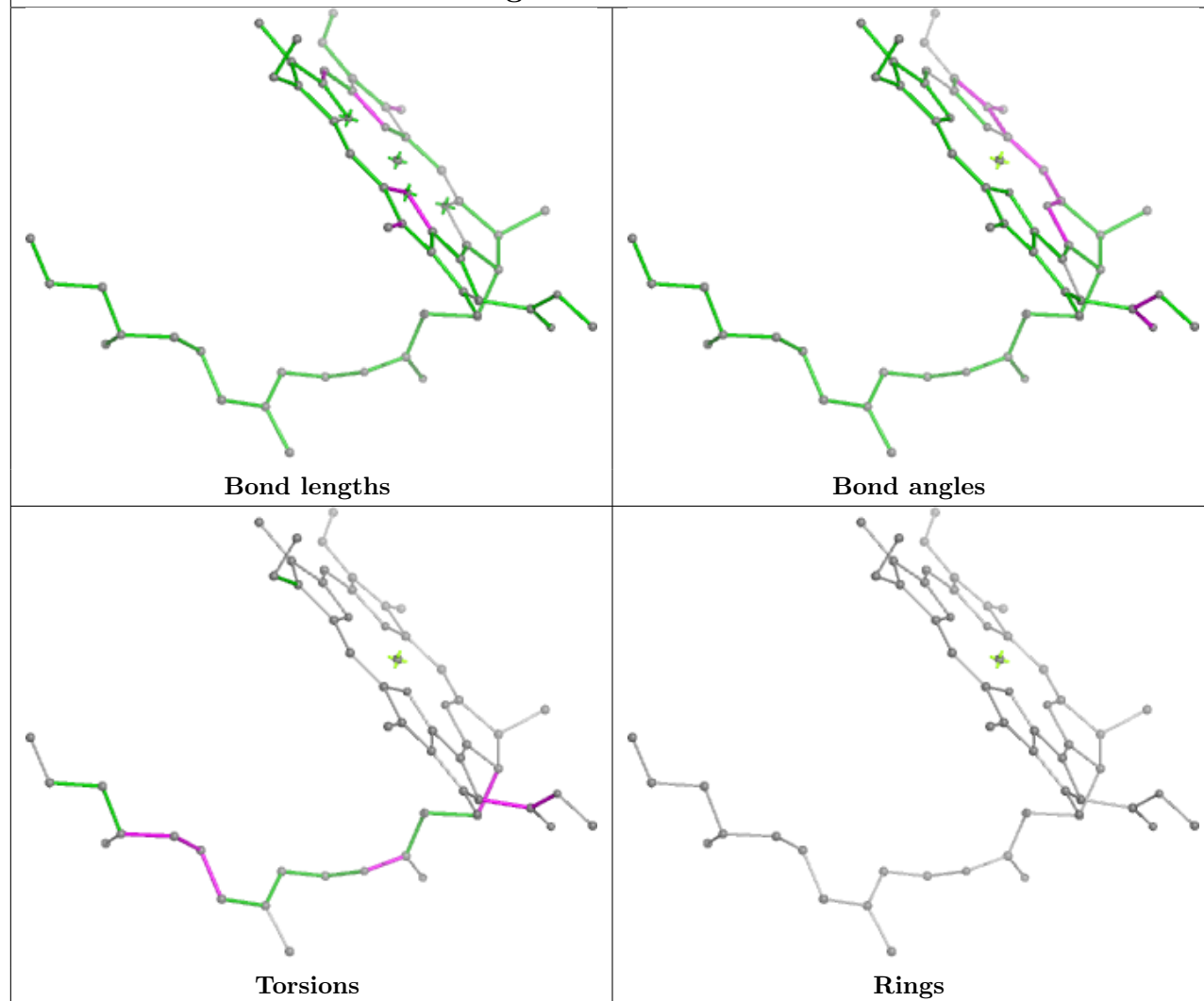




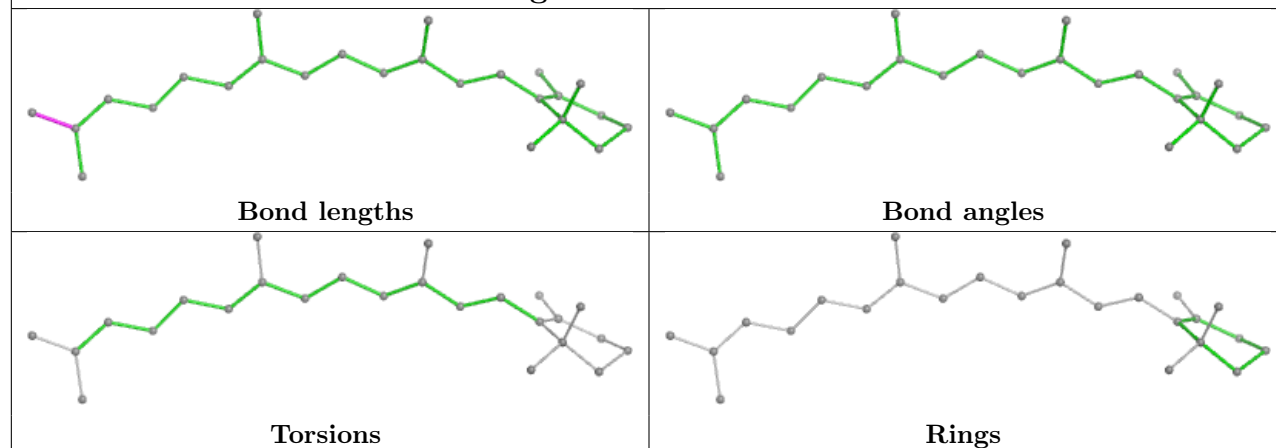




## Ligand CLA a 811

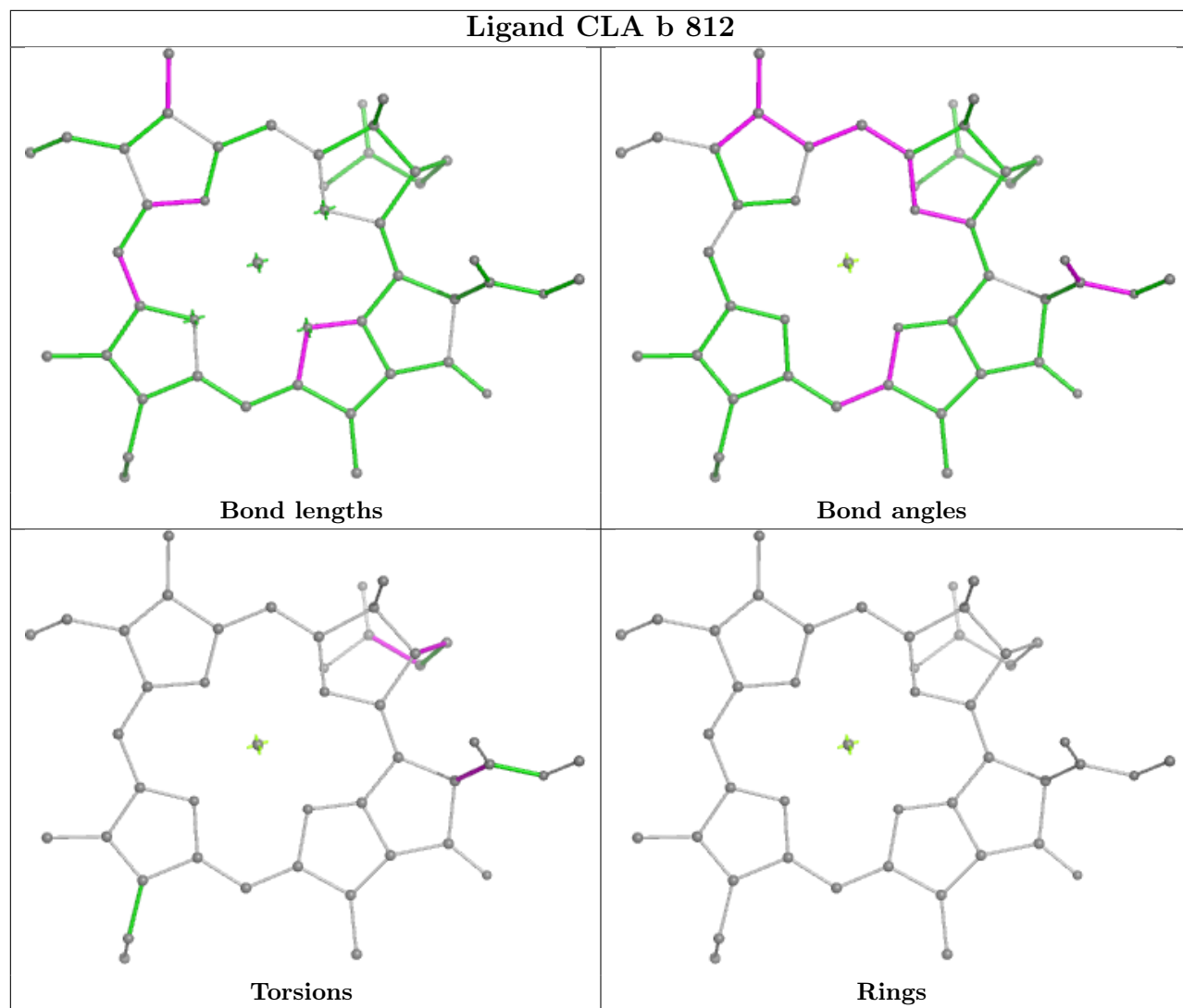


## Ligand BCR V 101

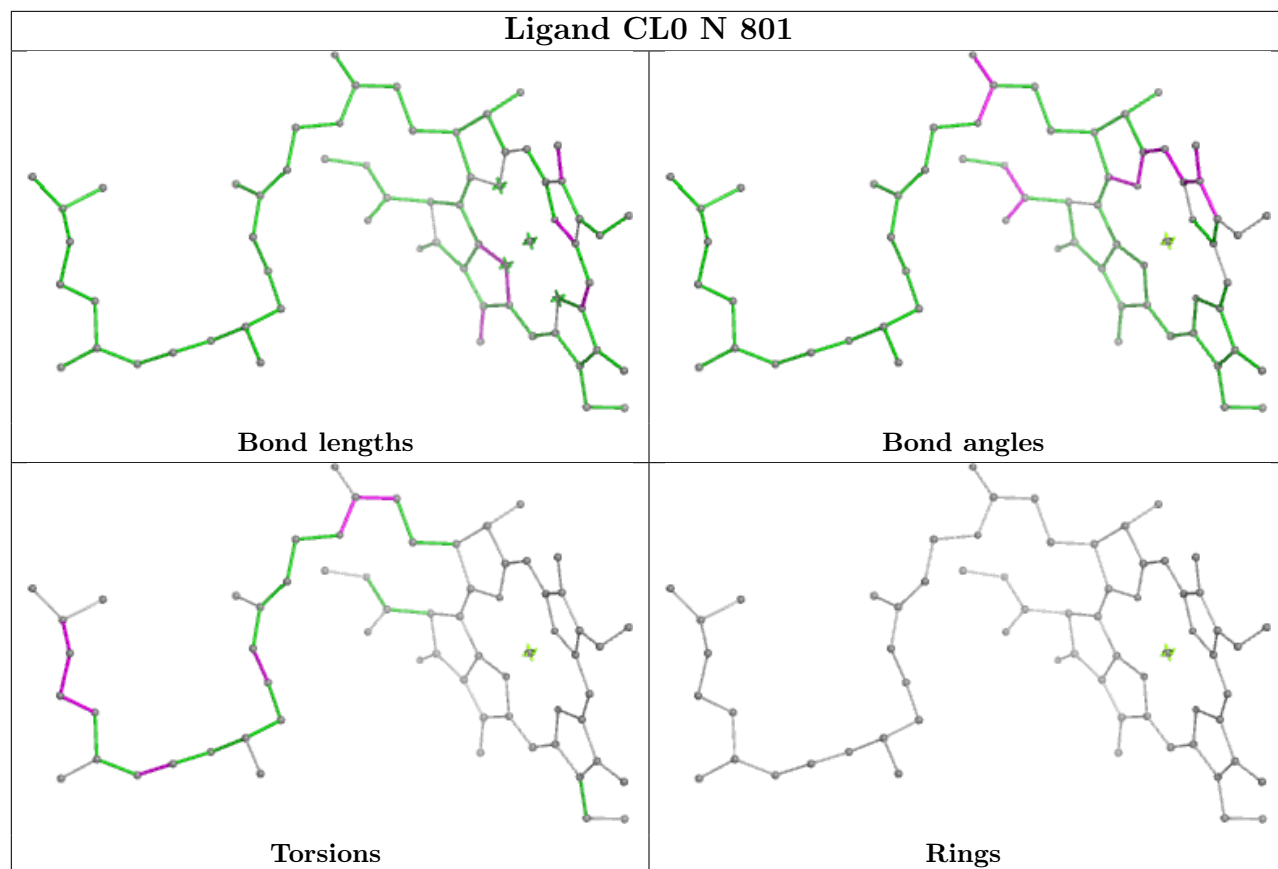




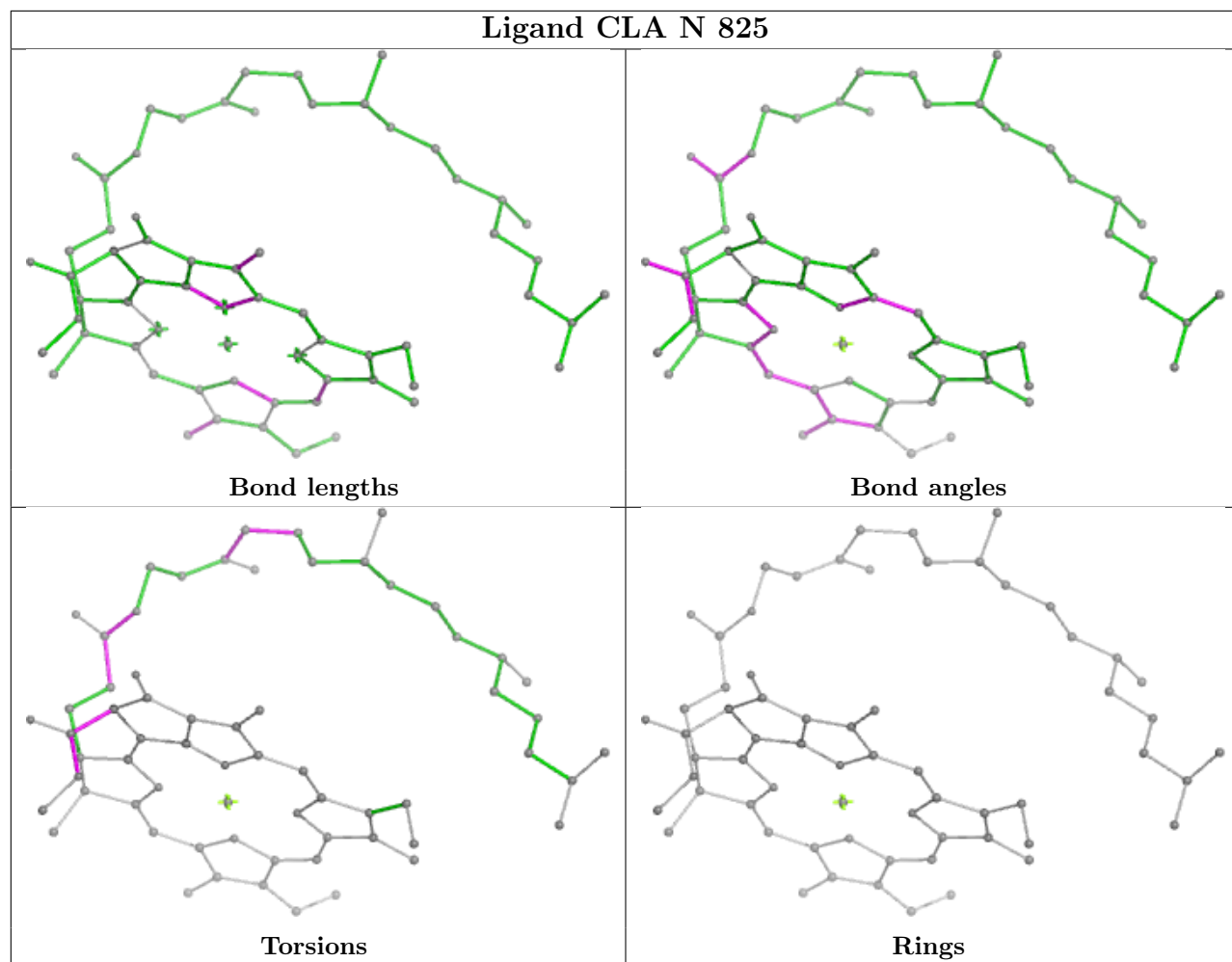
## Ligand CLA b 812





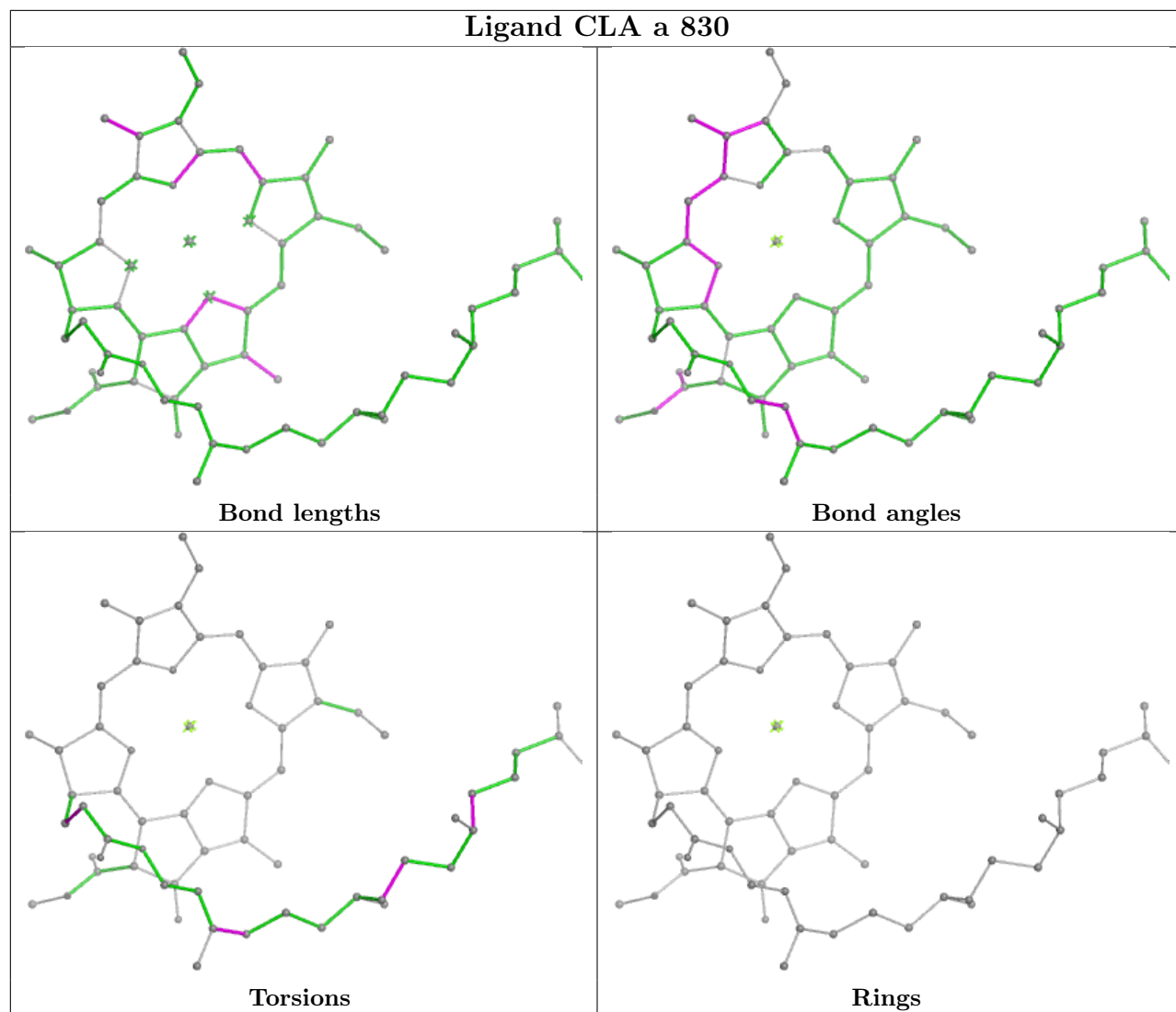






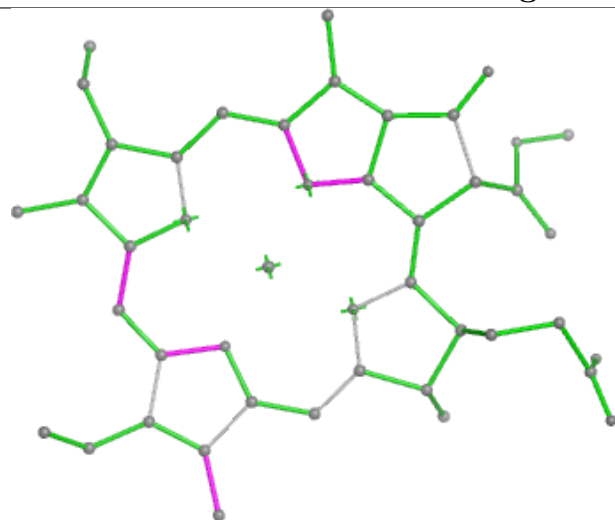


## Ligand CLA a 830

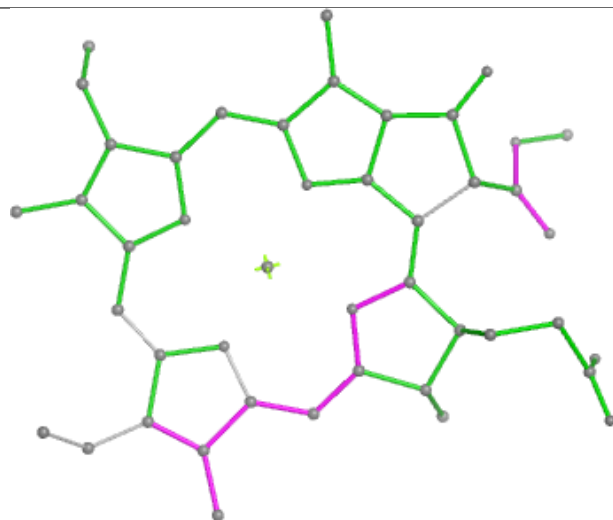




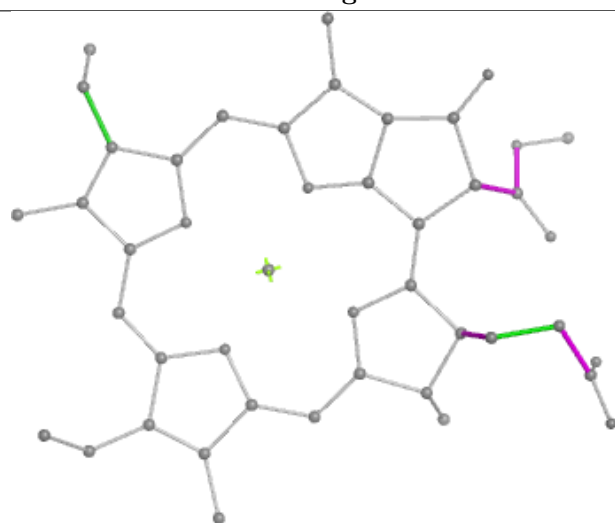
## Ligand CLA b 836



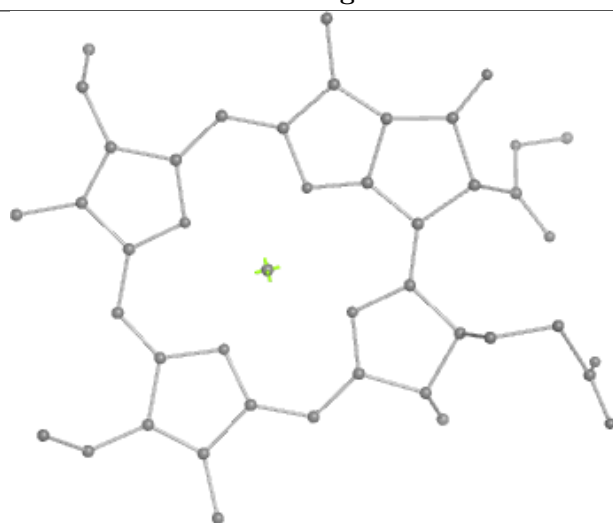
Bond lengths



Bond angles



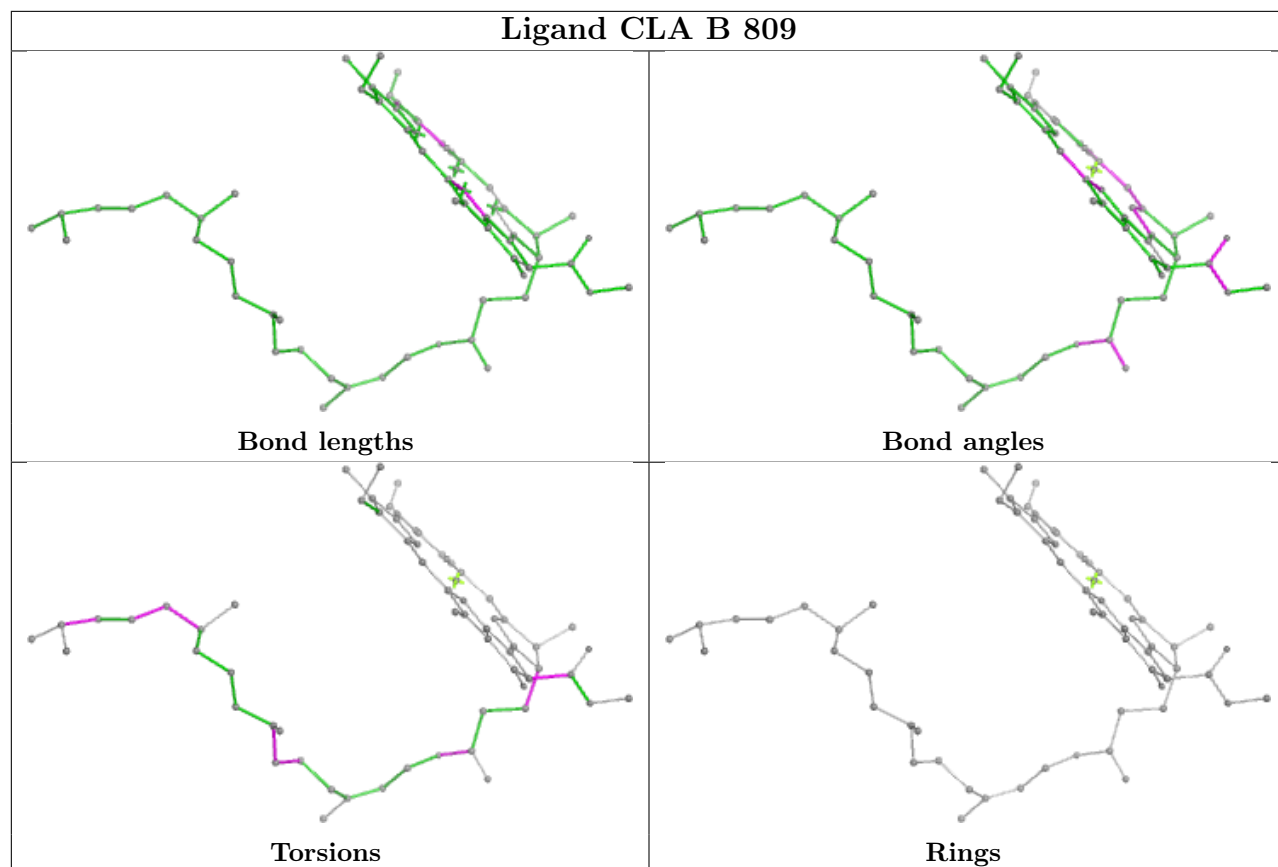
Torsions



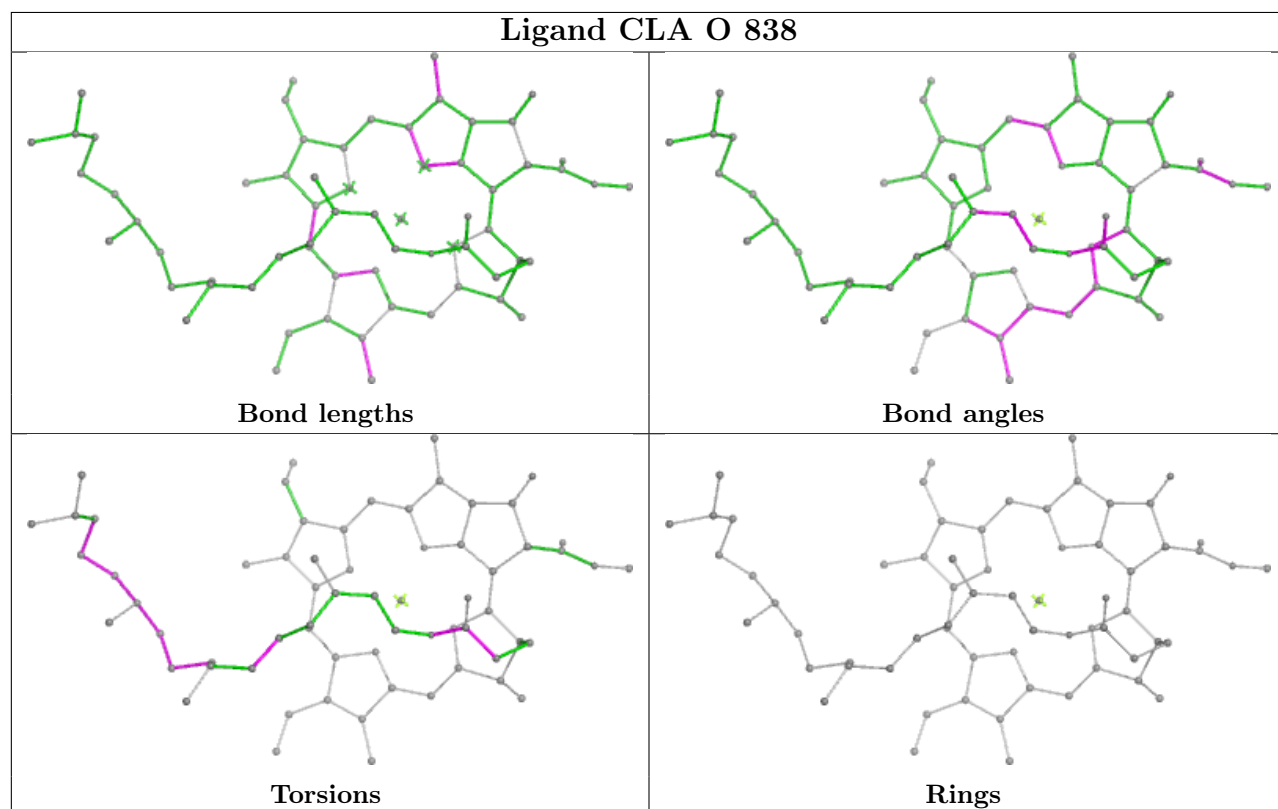
Rings



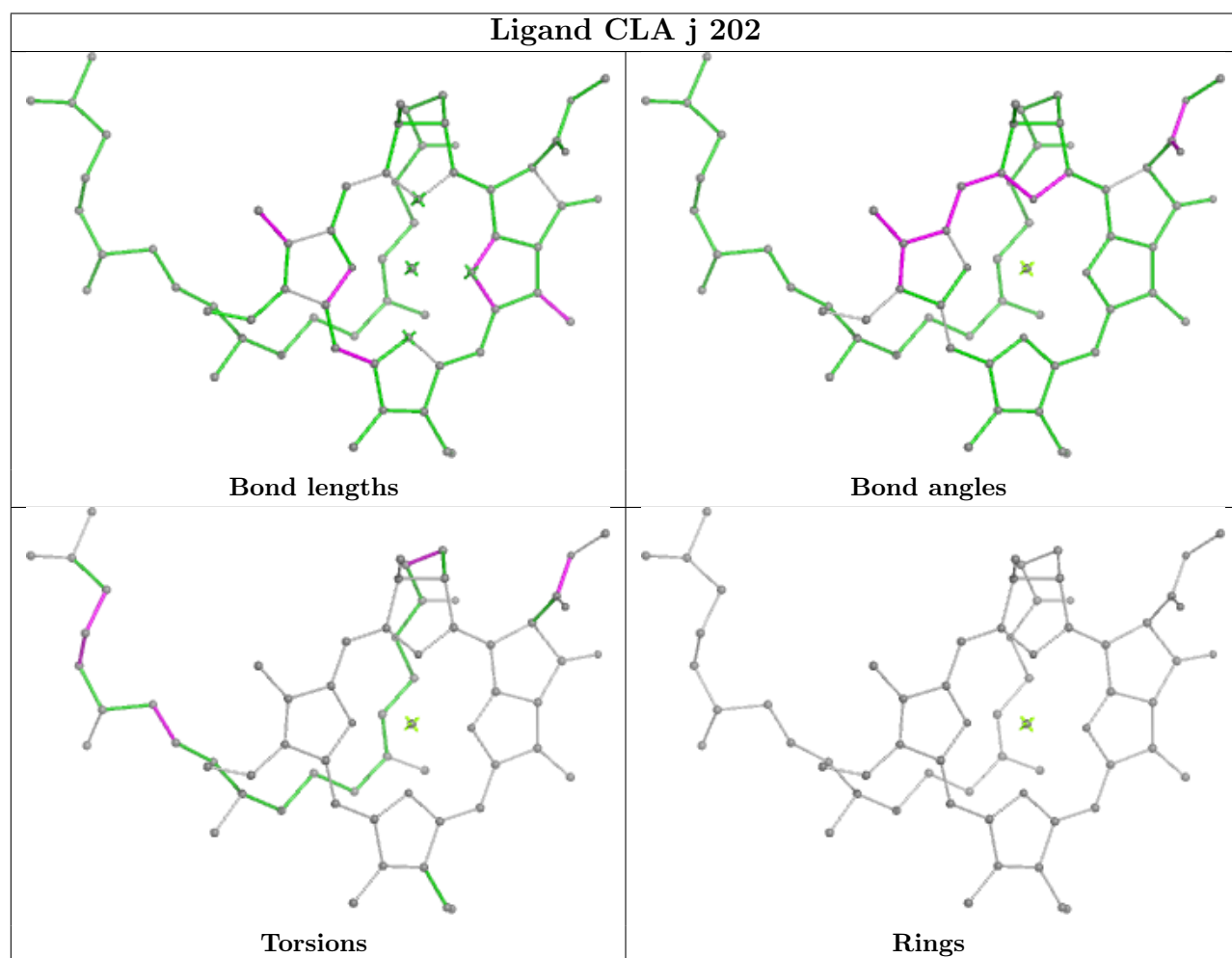
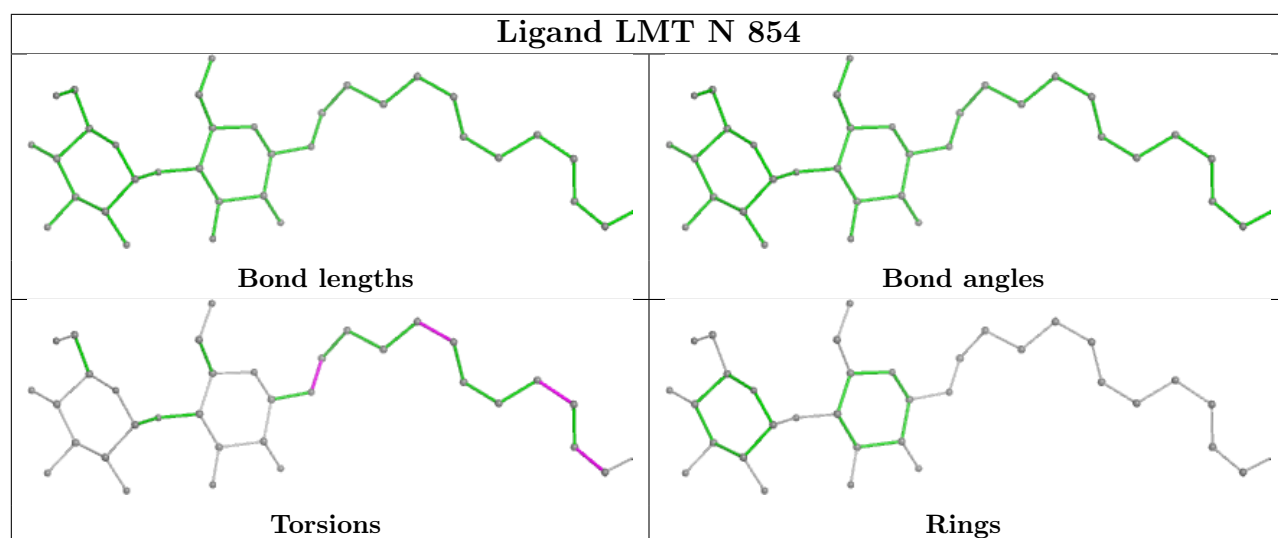
## Ligand CLA B 809



## Ligand CLA O 838

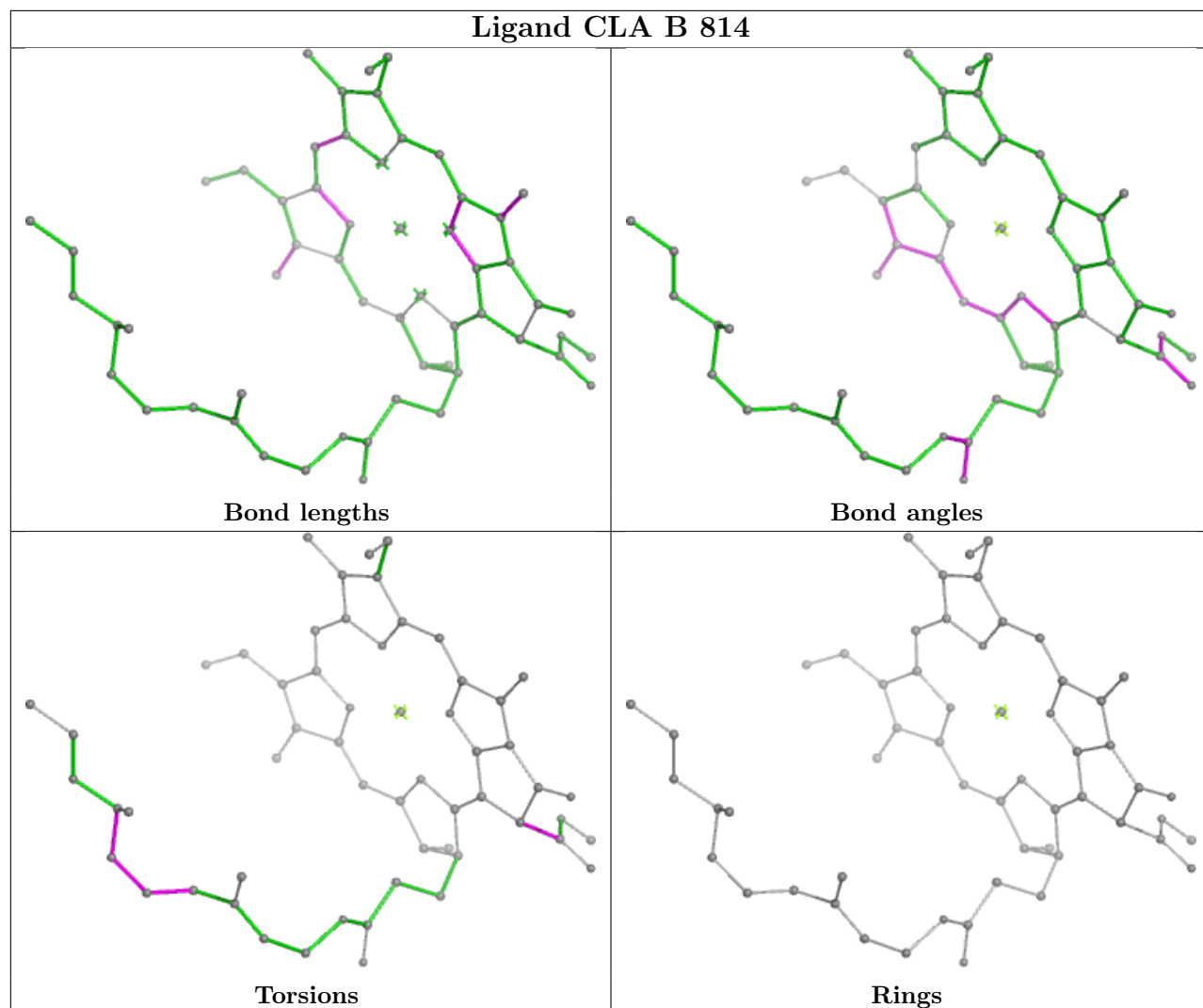




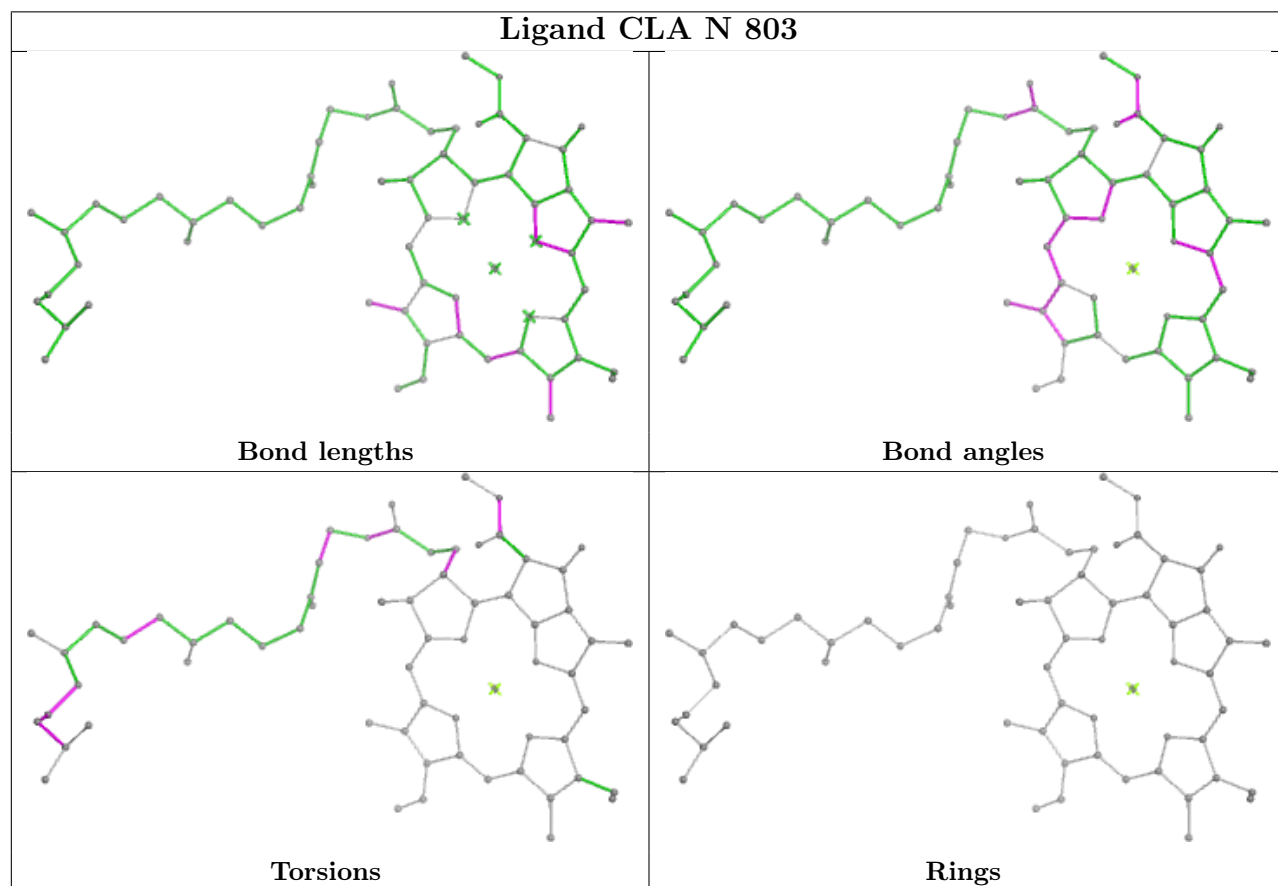
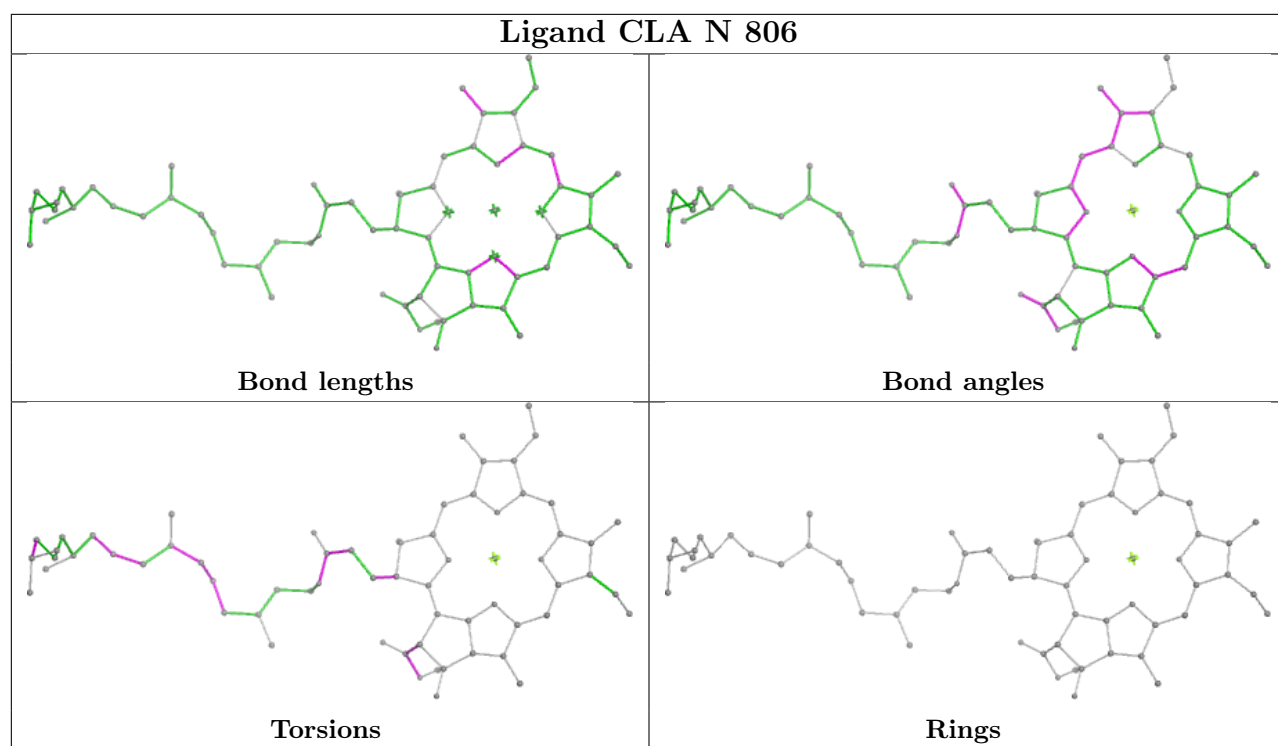




## Ligand CLA B 814

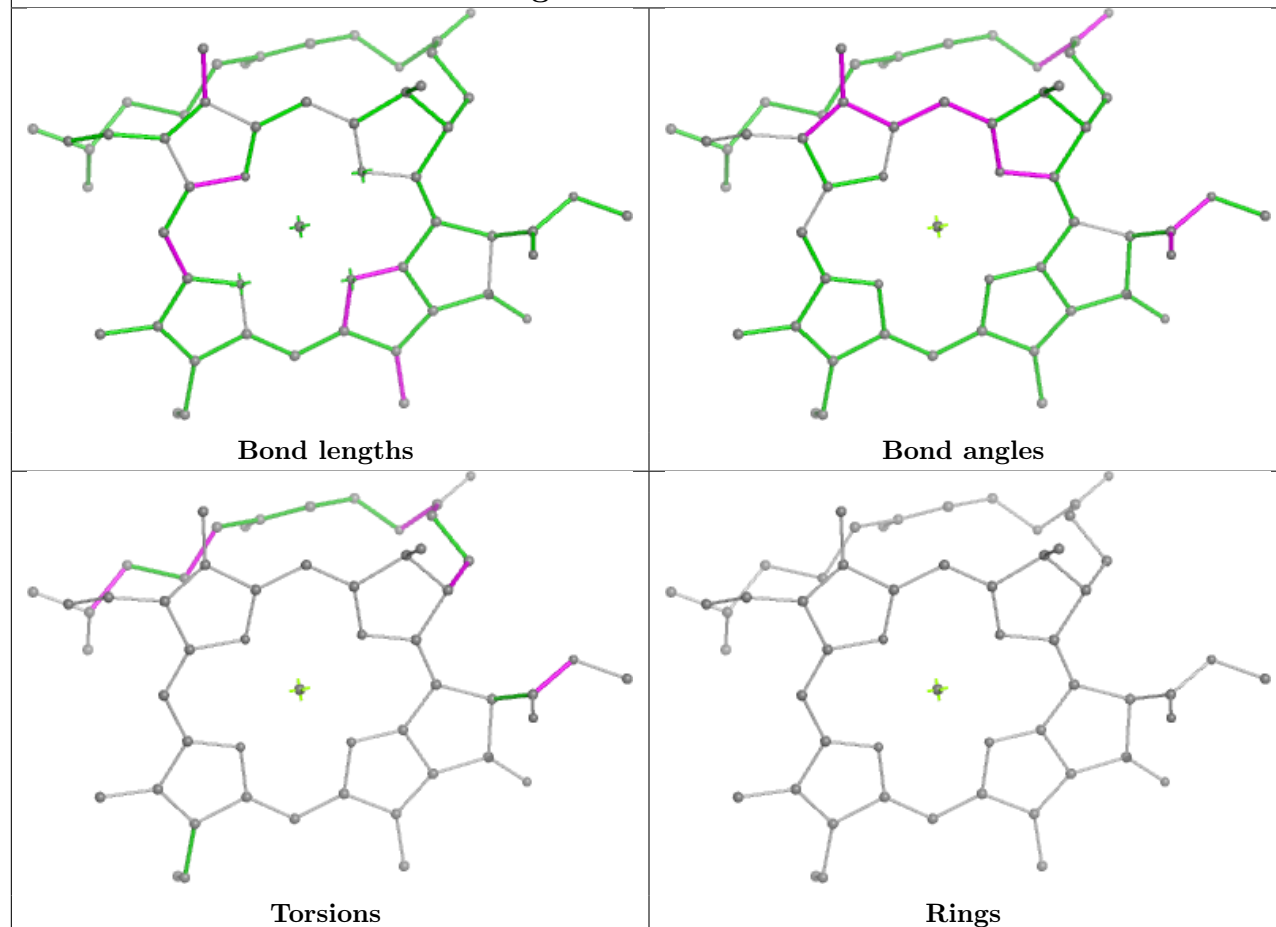




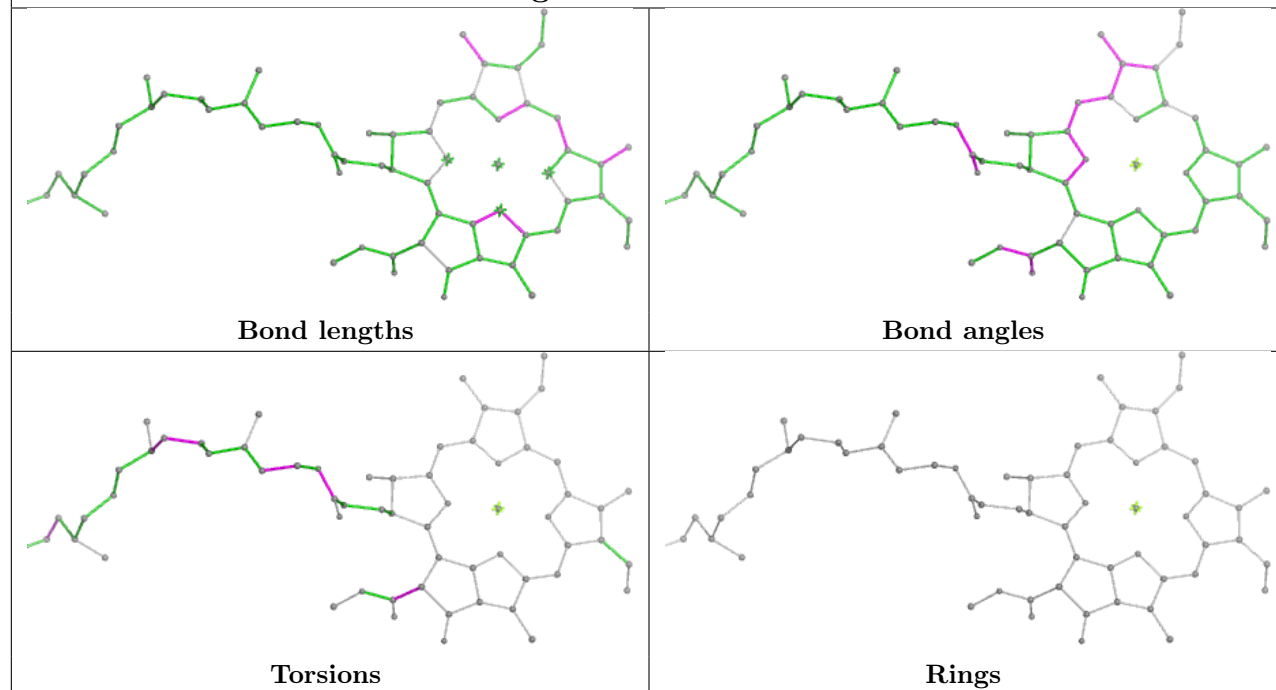




## Ligand CLA O 820

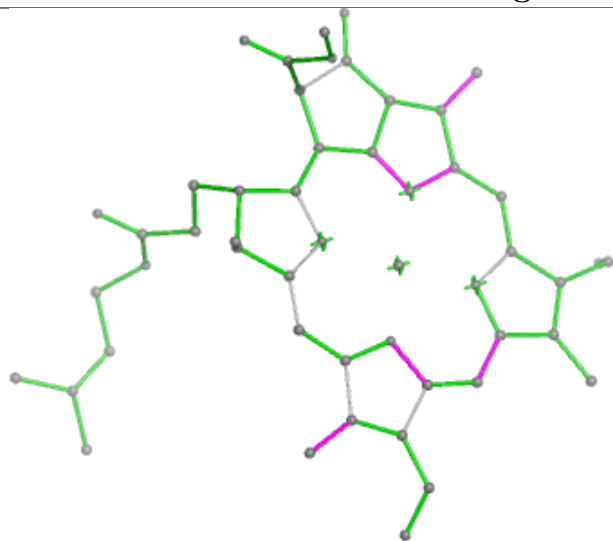


## Ligand CLA A 828

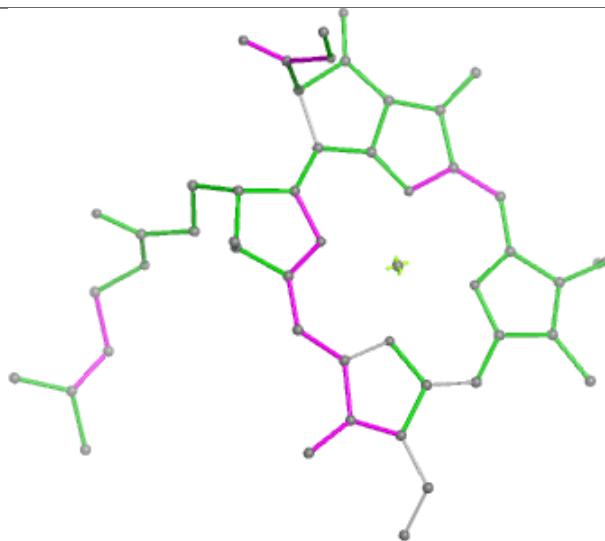




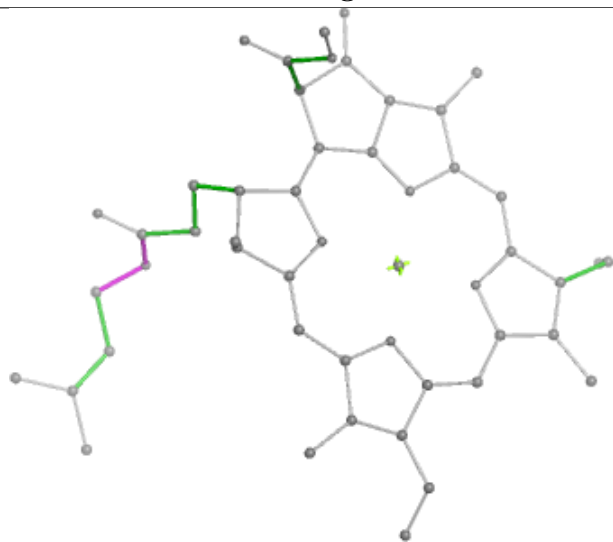
## Ligand CLA N 832



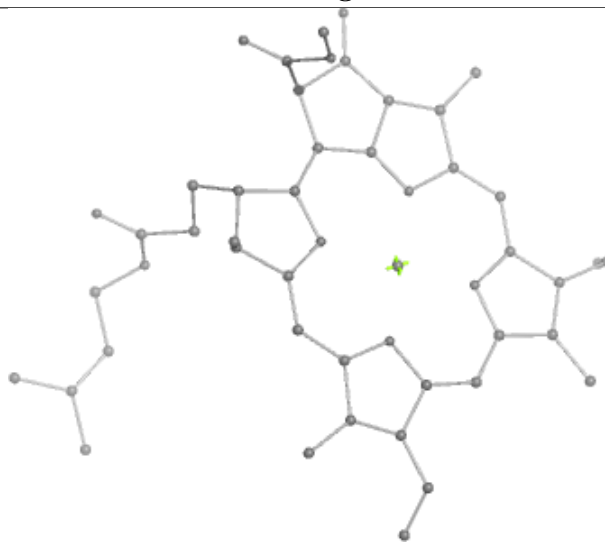
Bond lengths



Bond angles

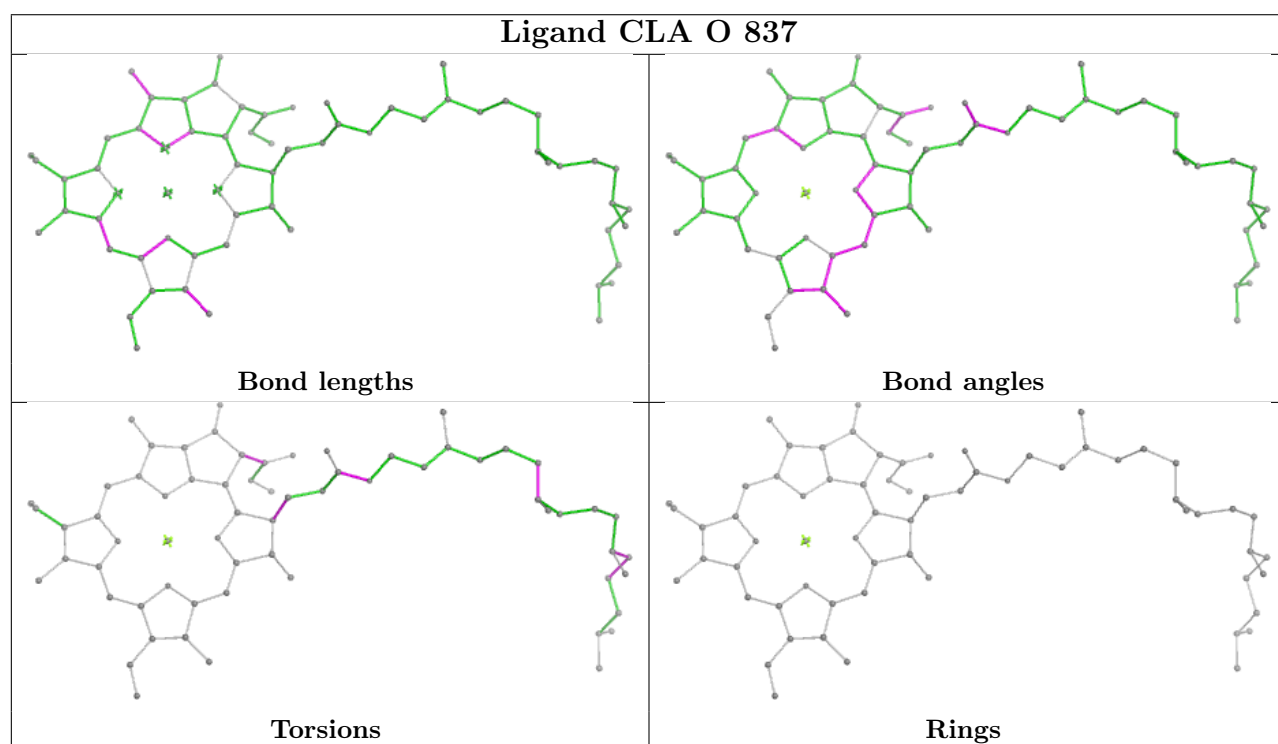
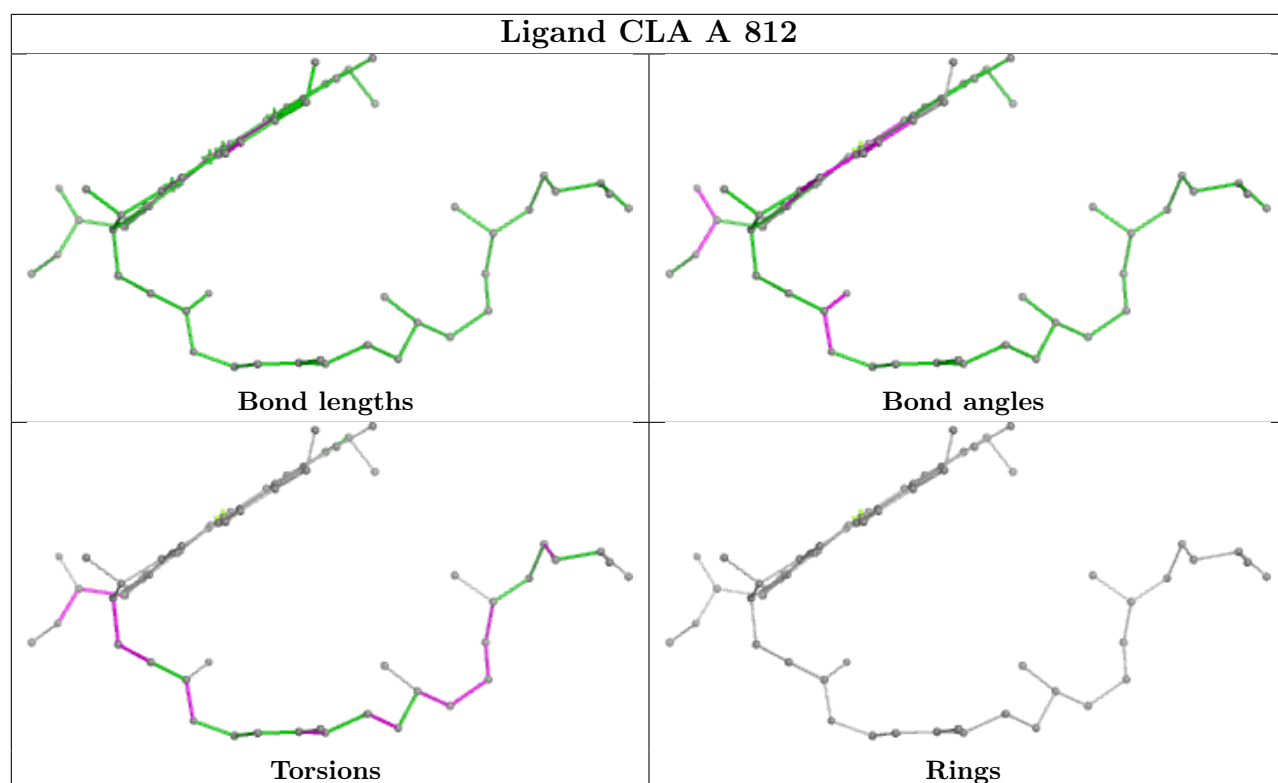


Torsions

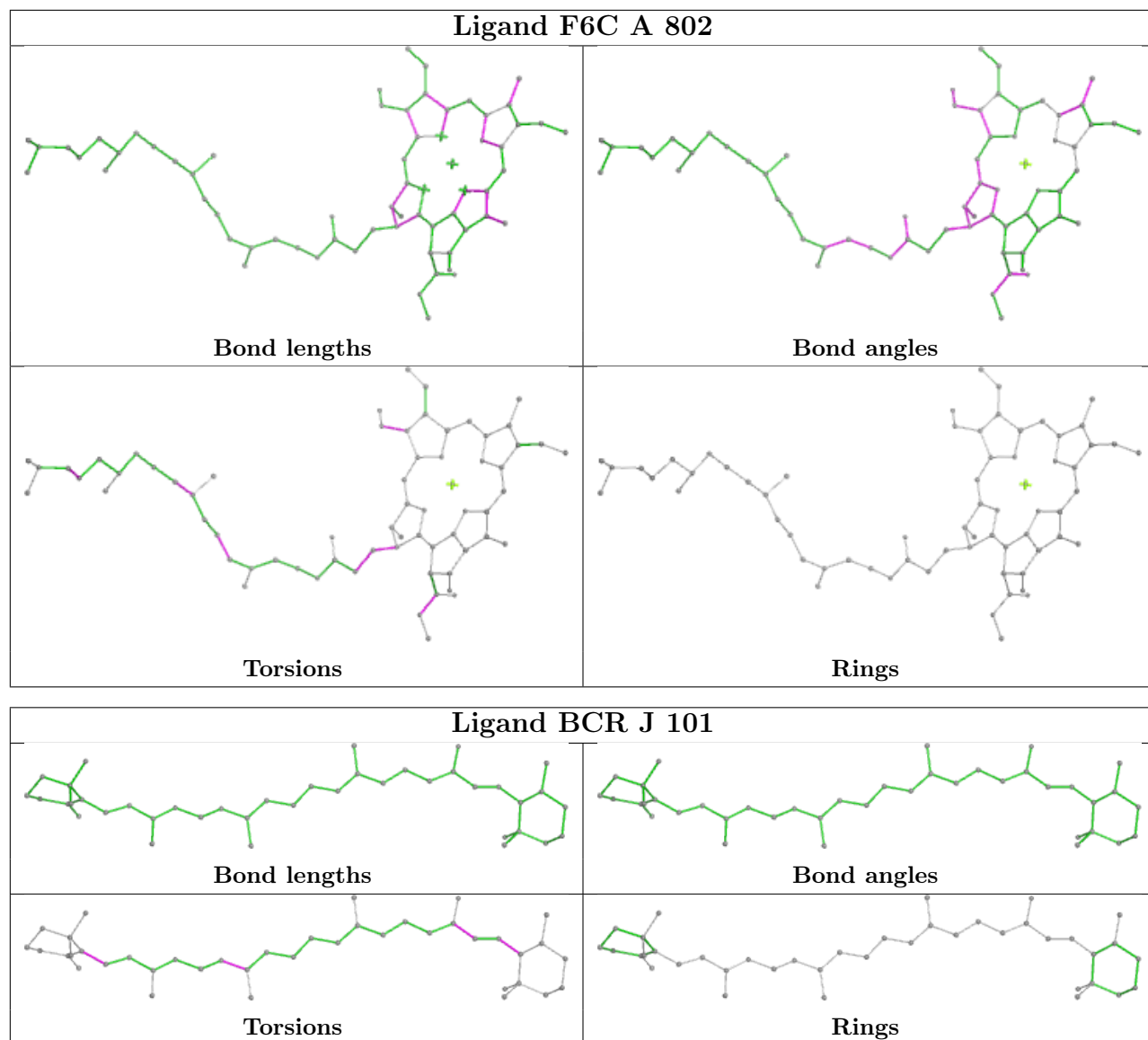


Rings

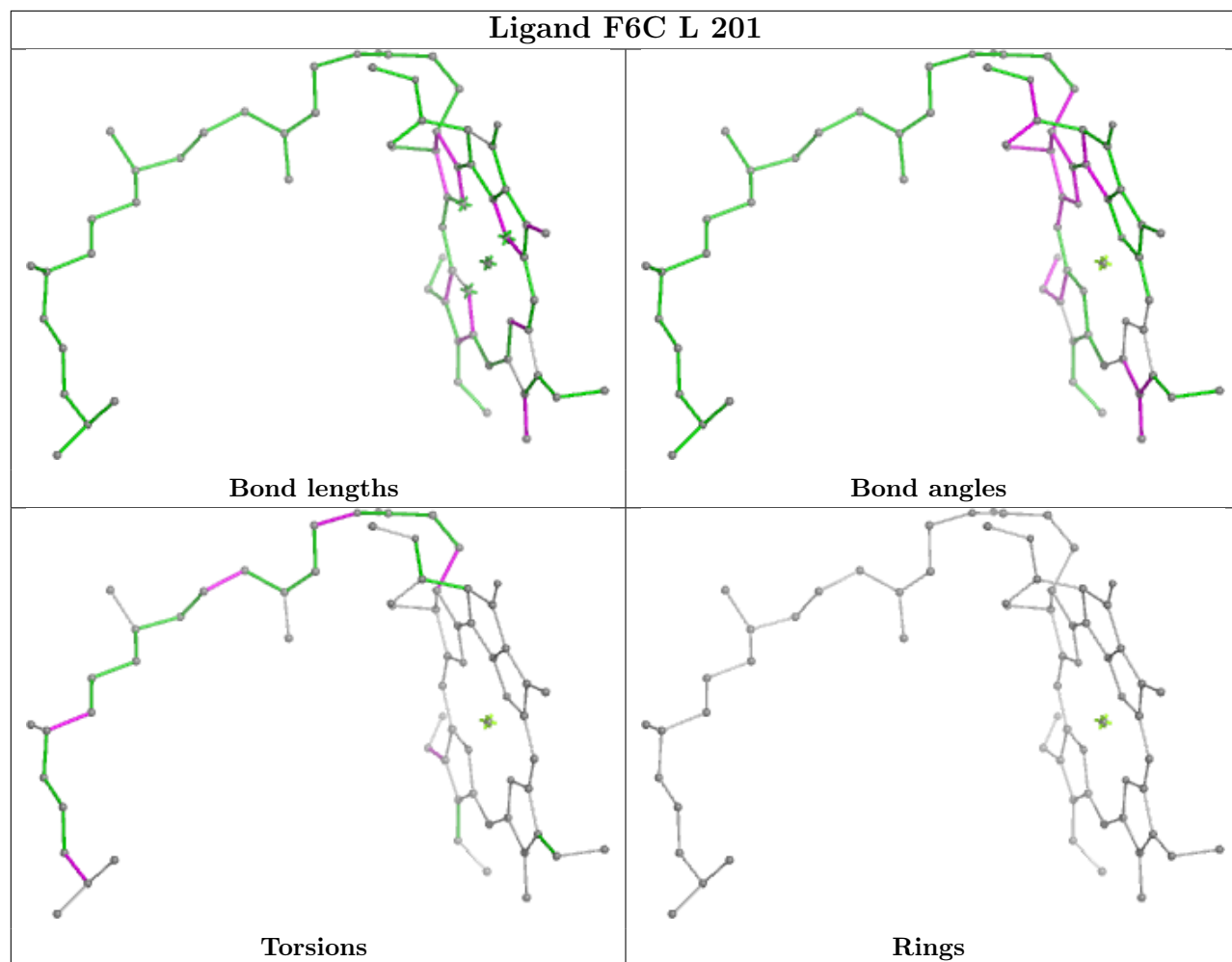




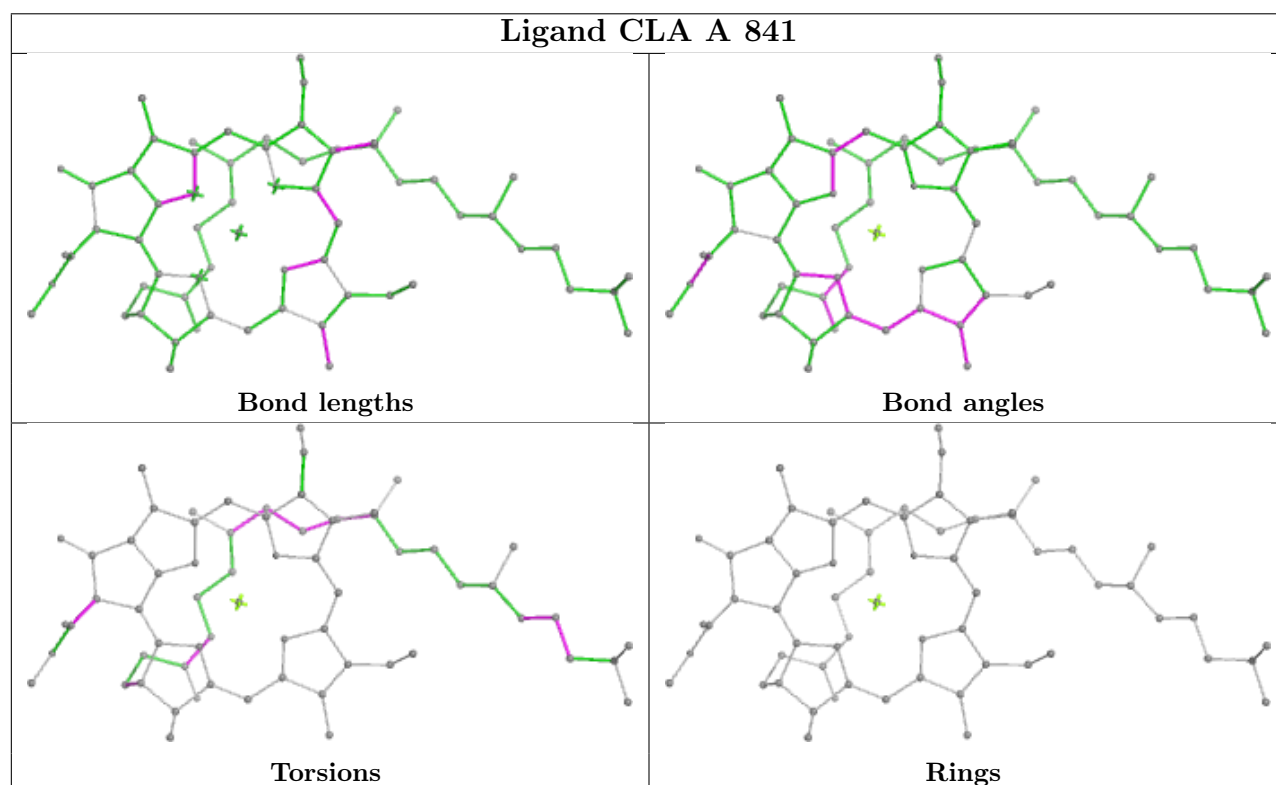
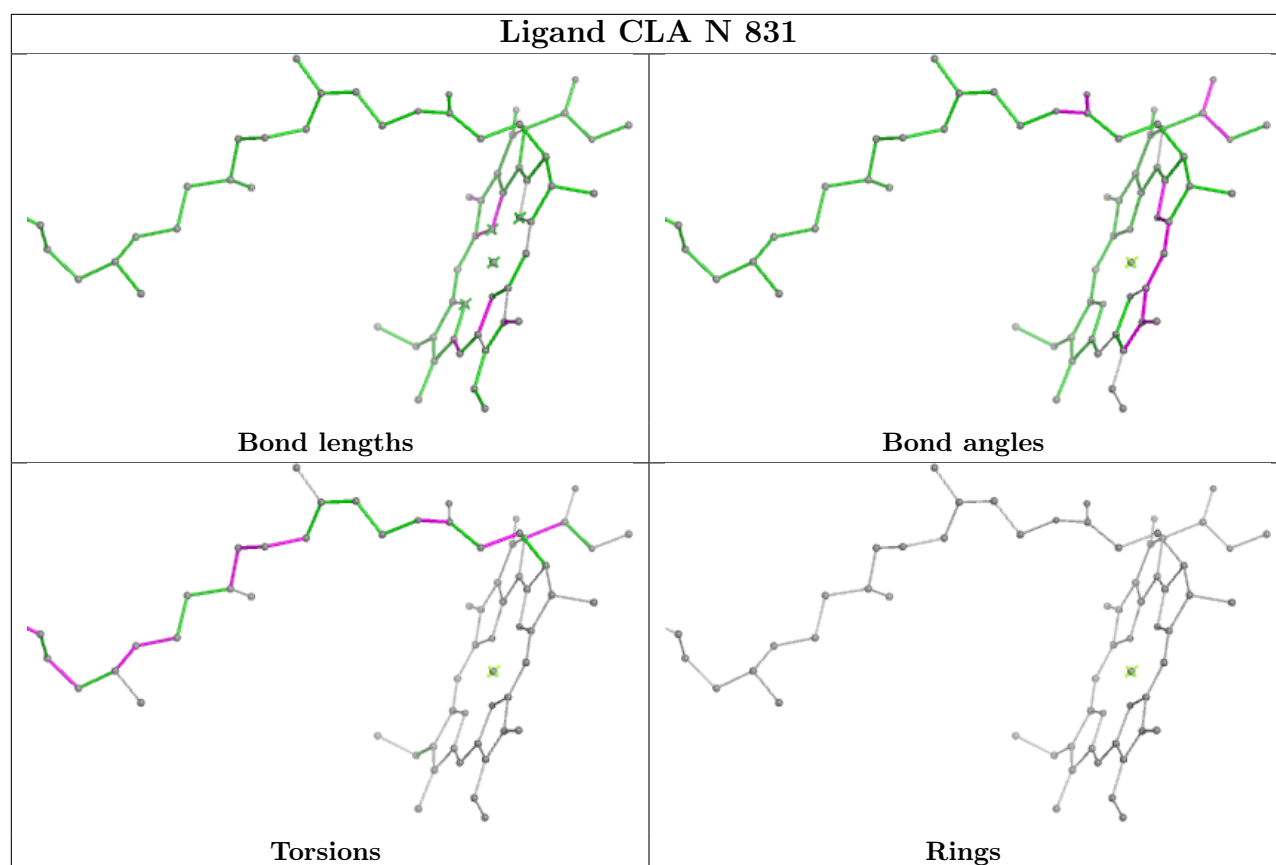




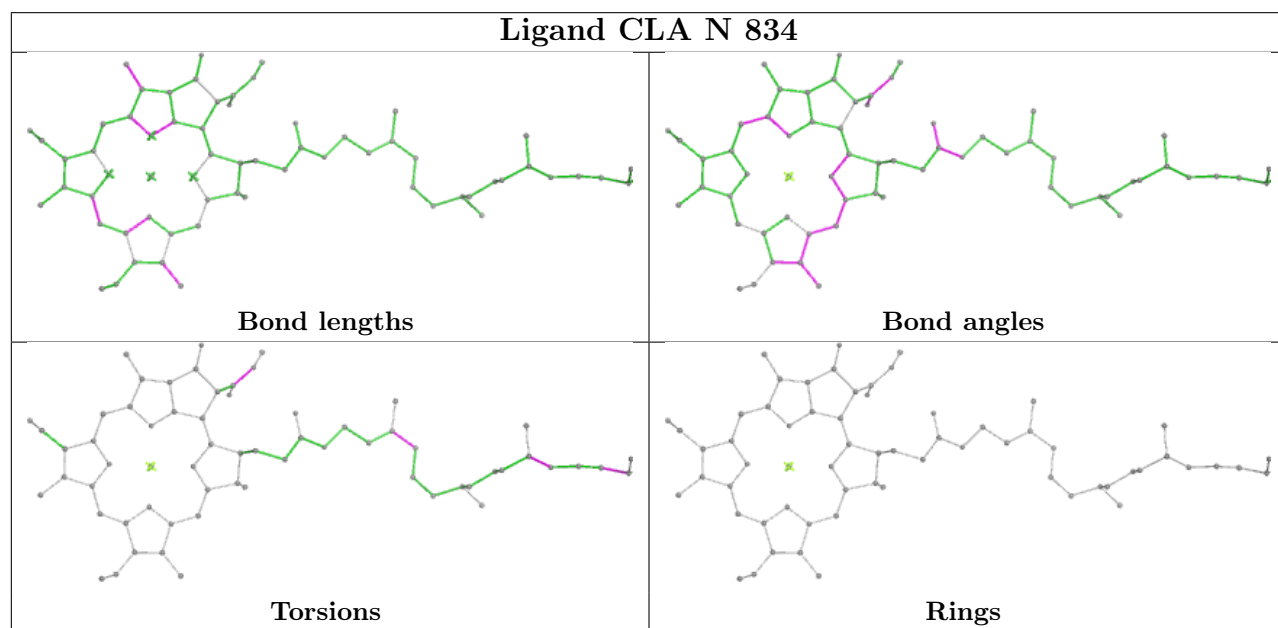
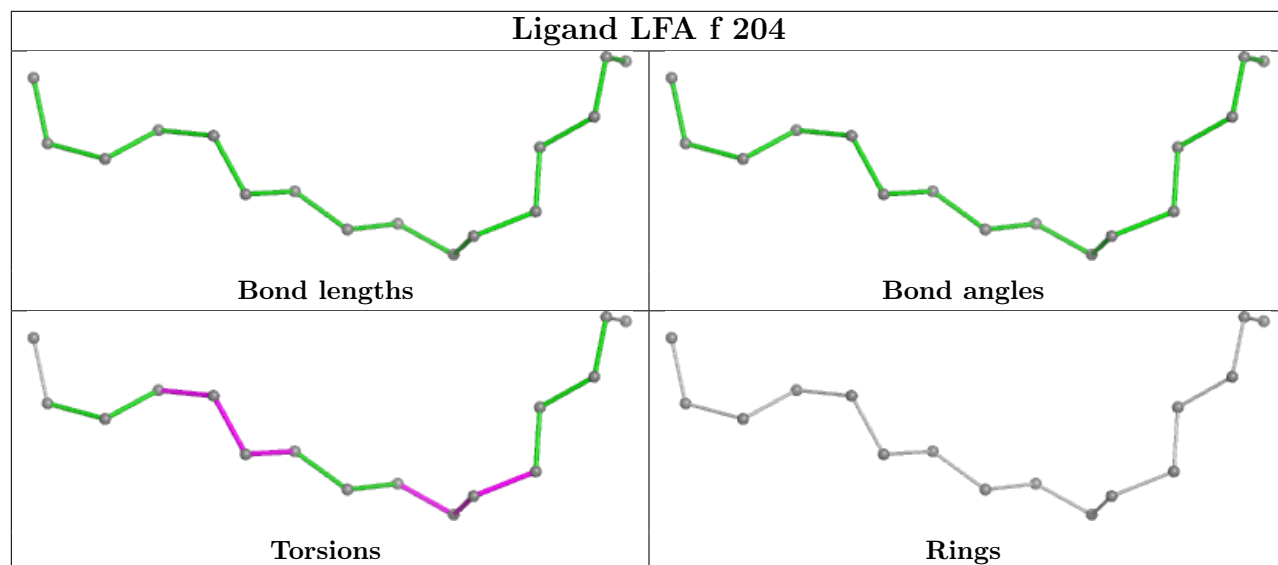






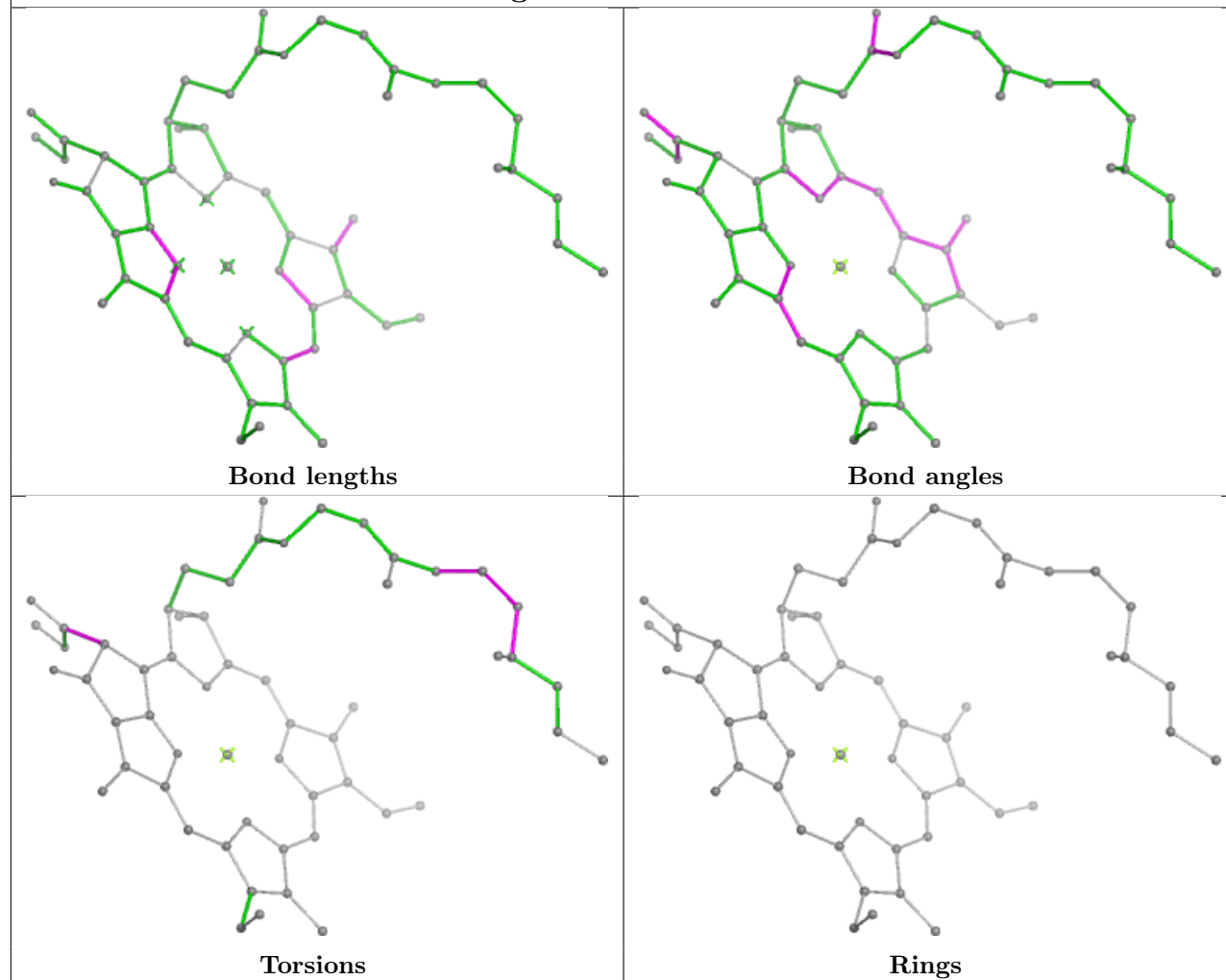




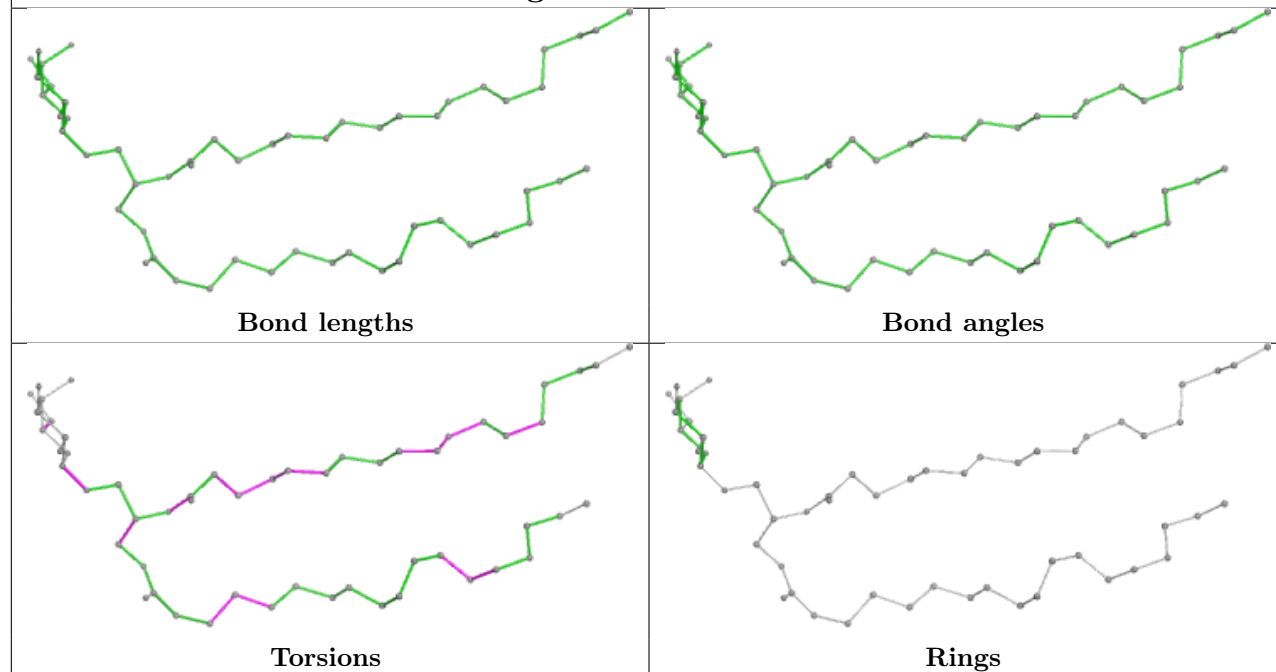




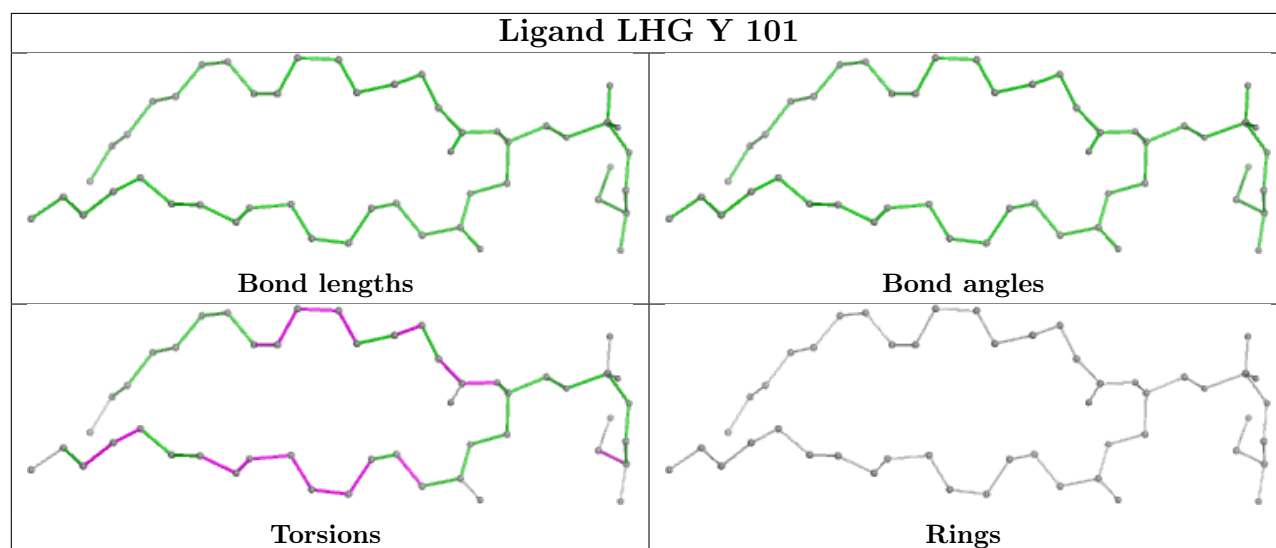
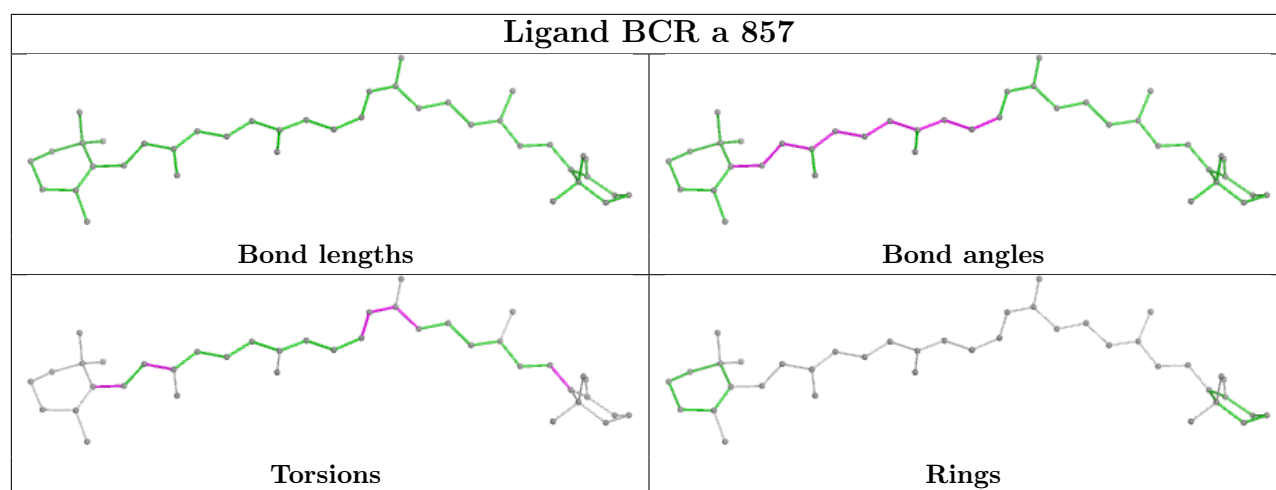
## Ligand CLA O 816



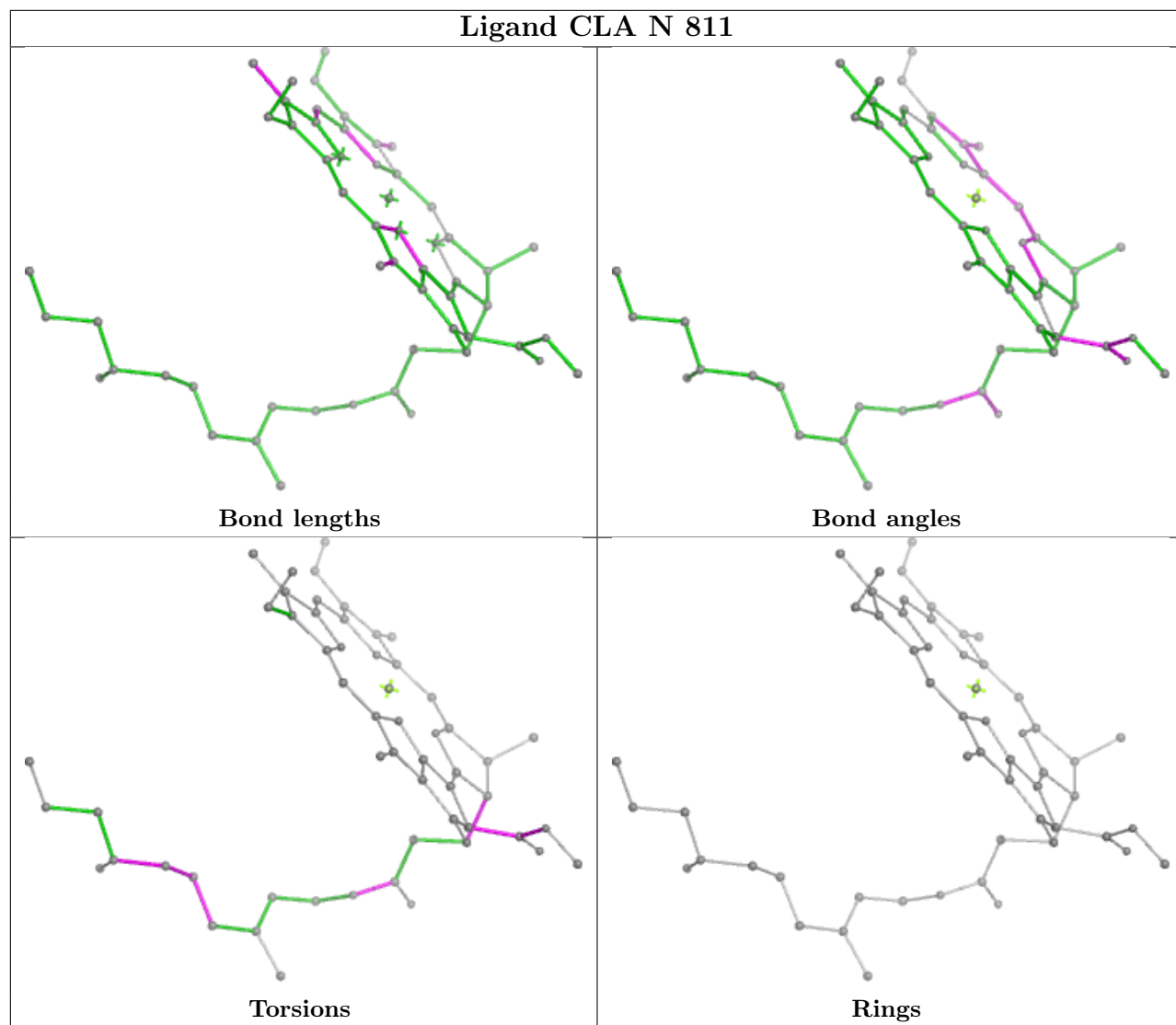
## Ligand LMG U 102



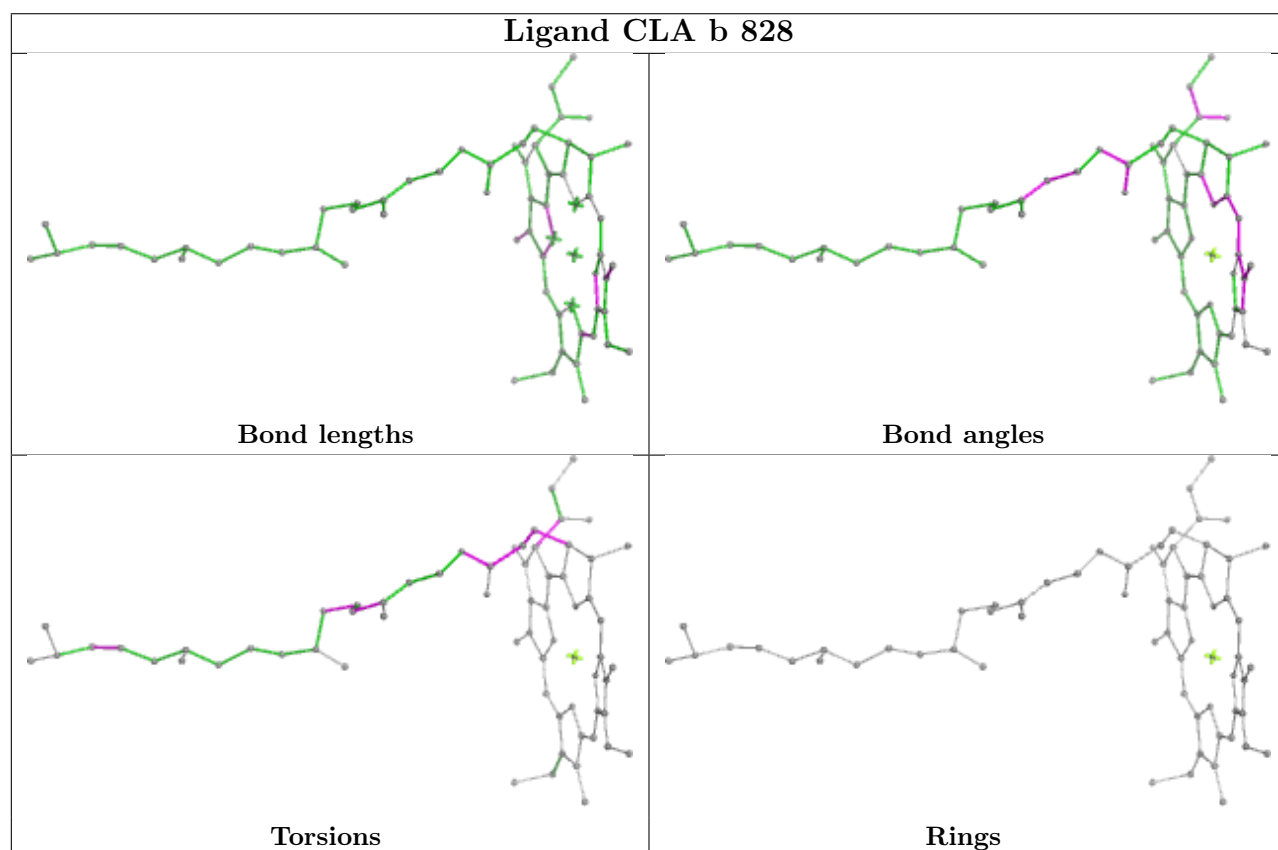
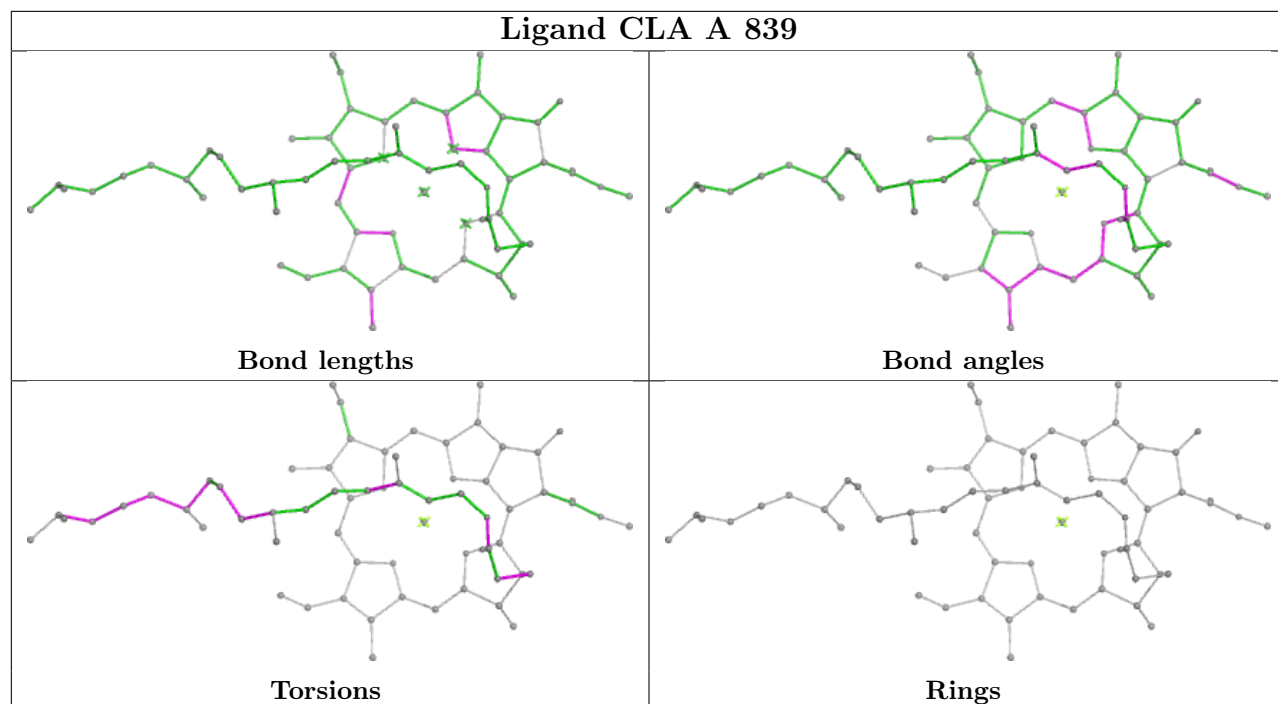




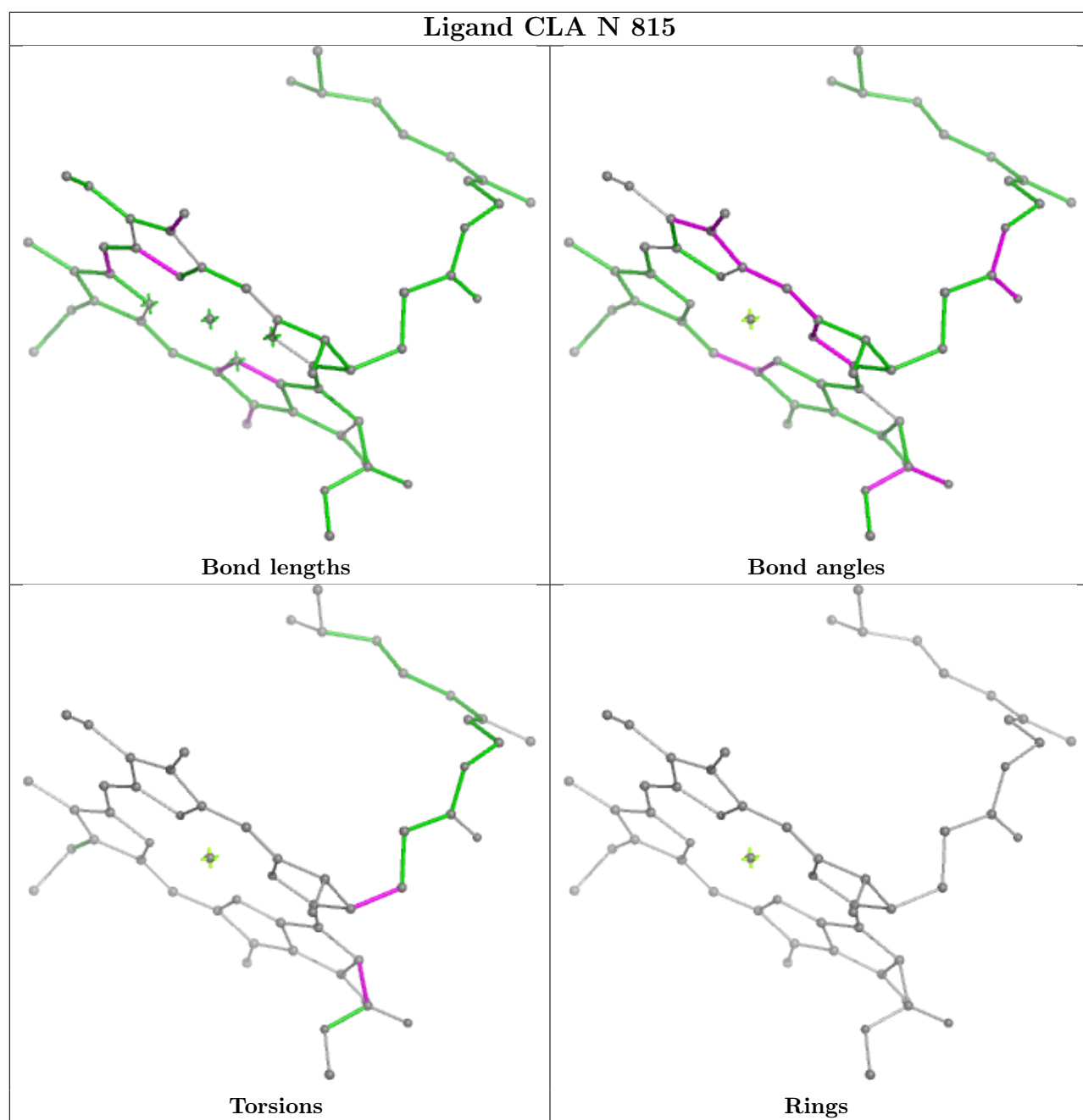




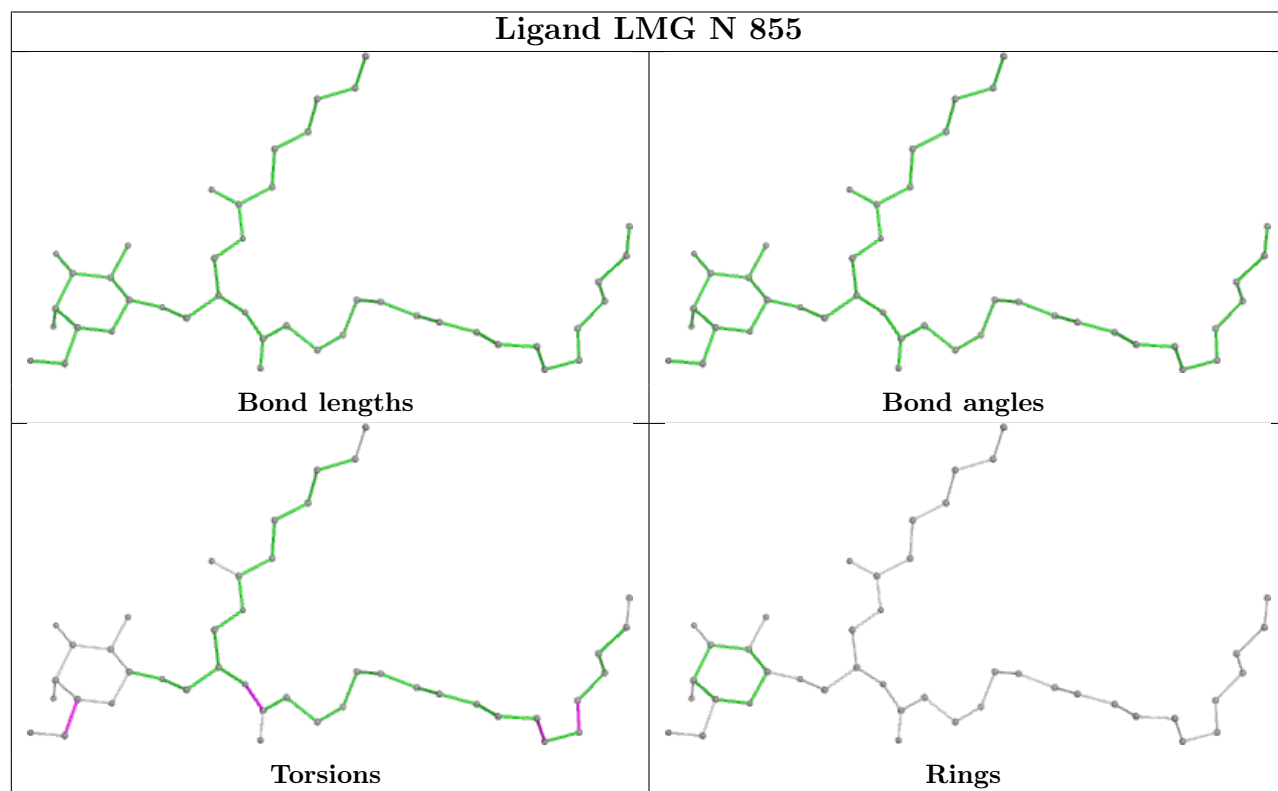
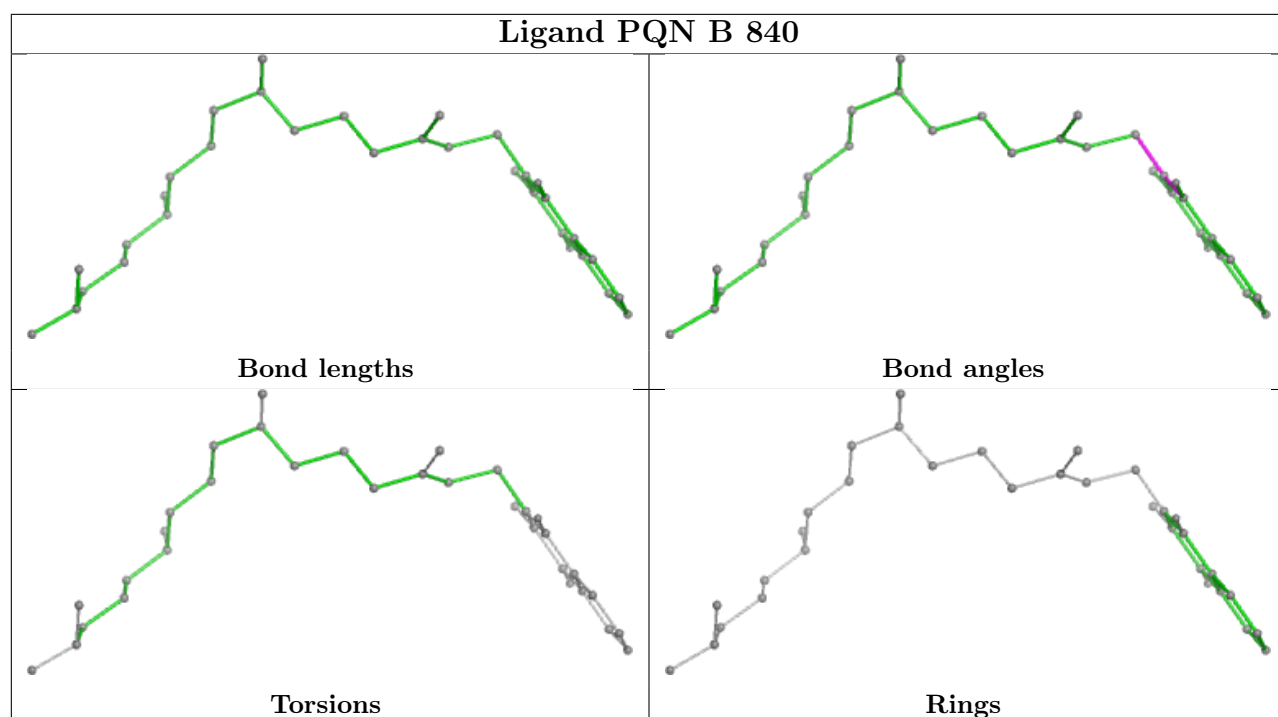




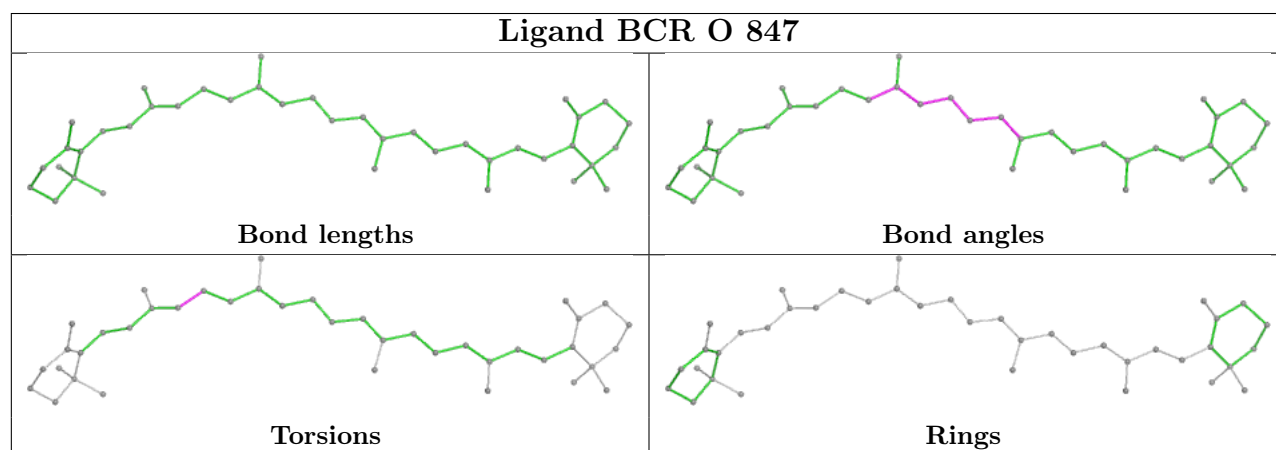
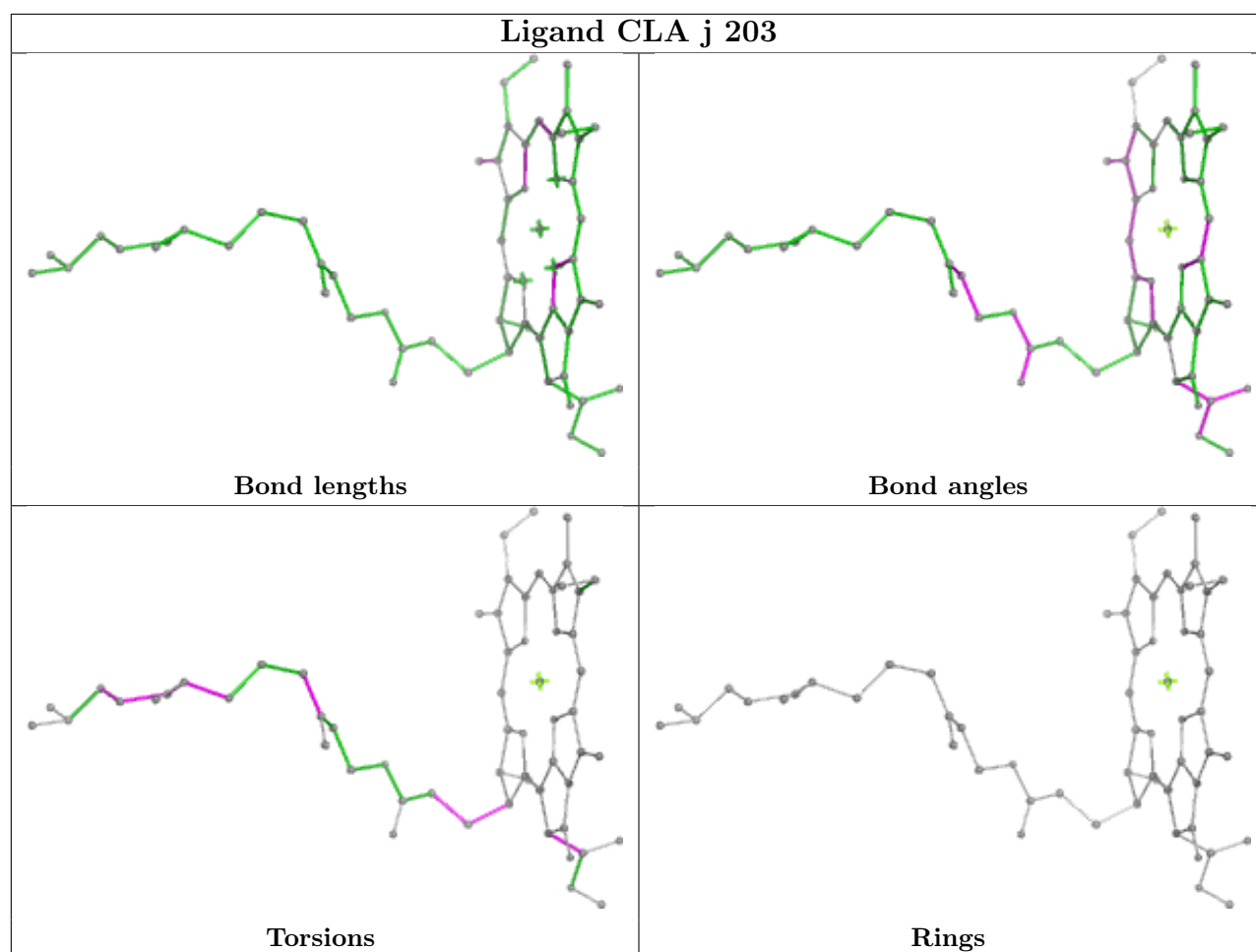




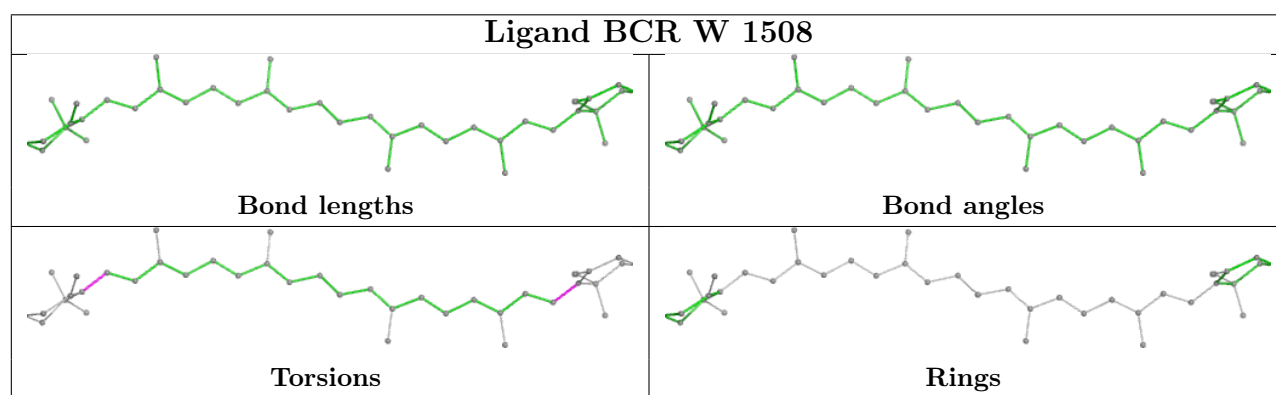
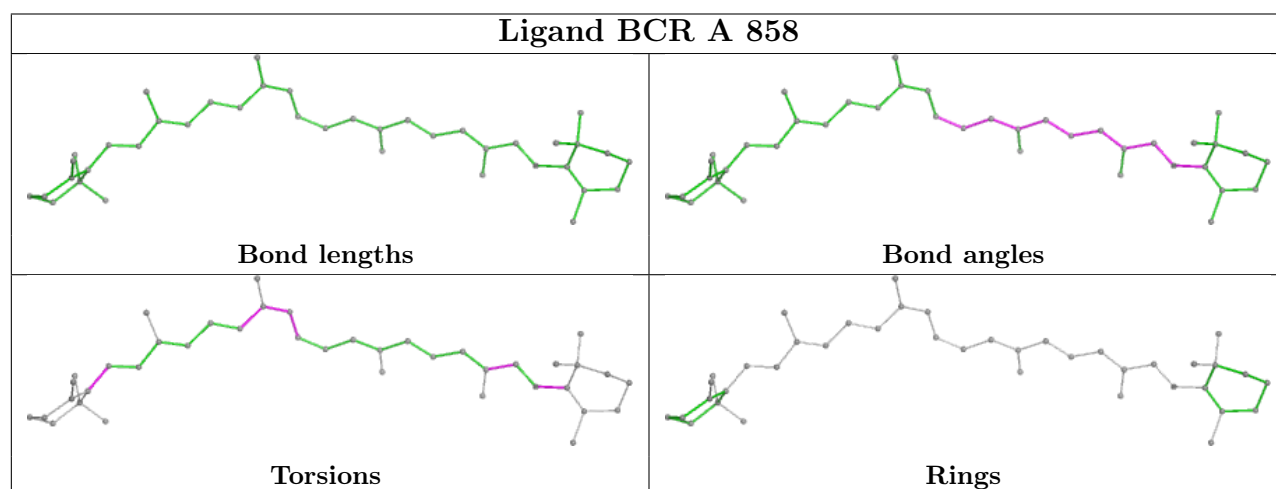
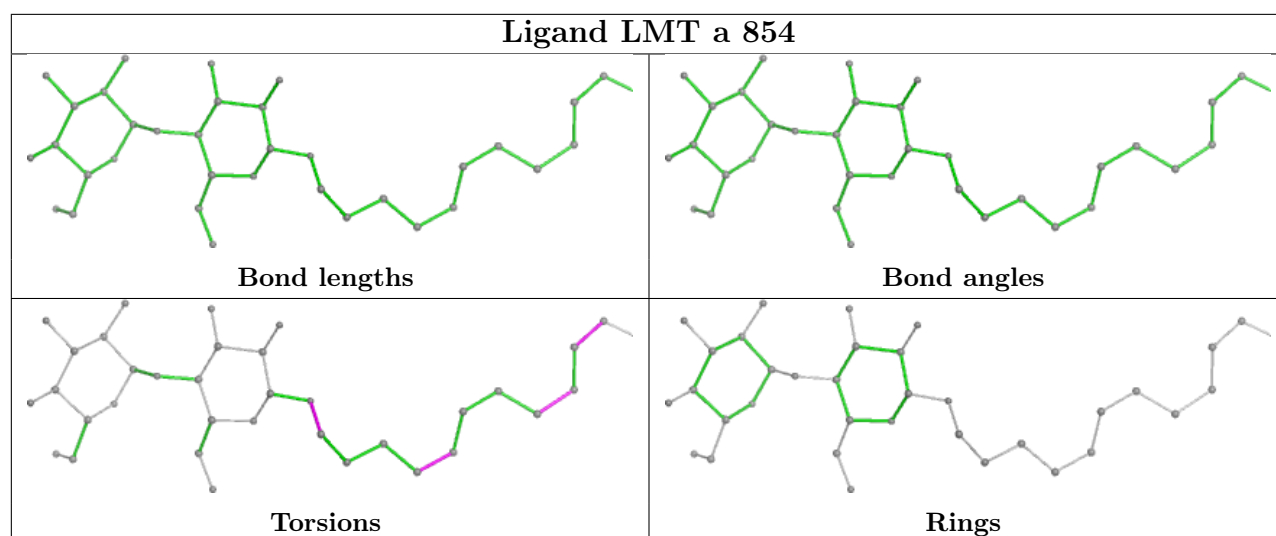




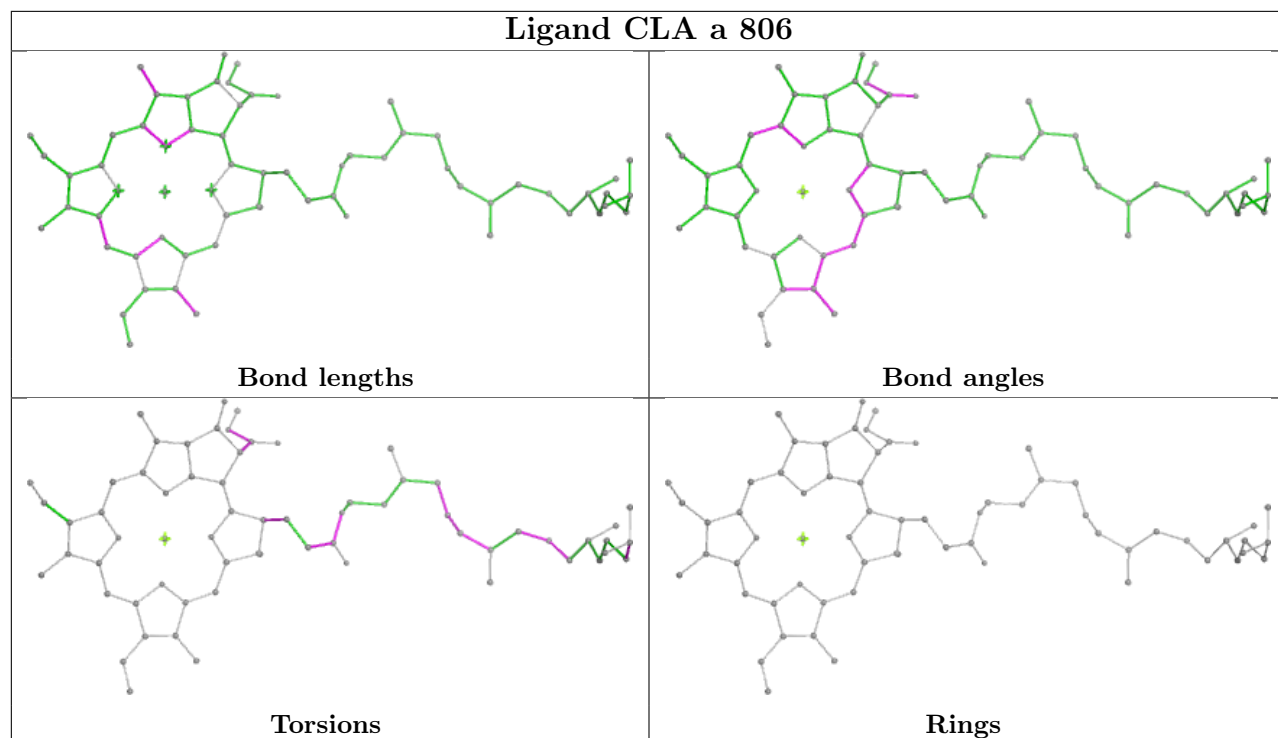
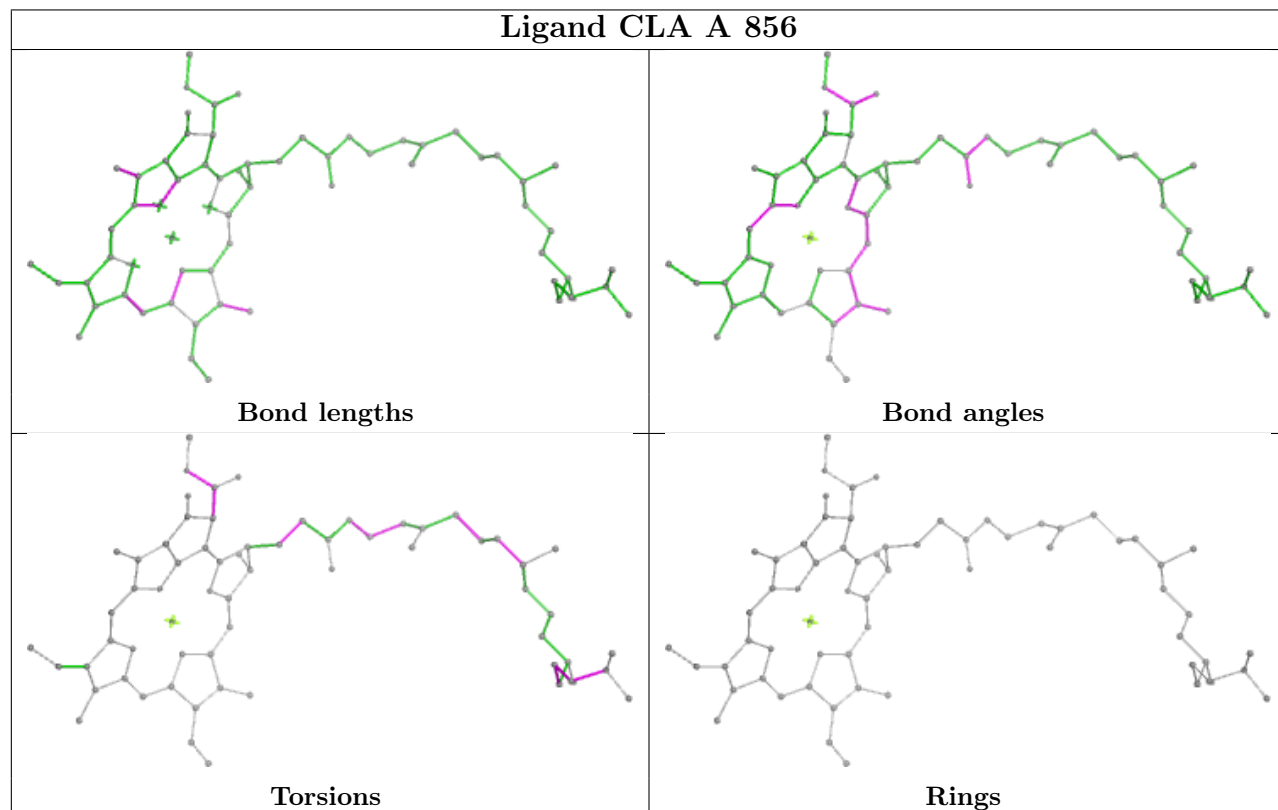






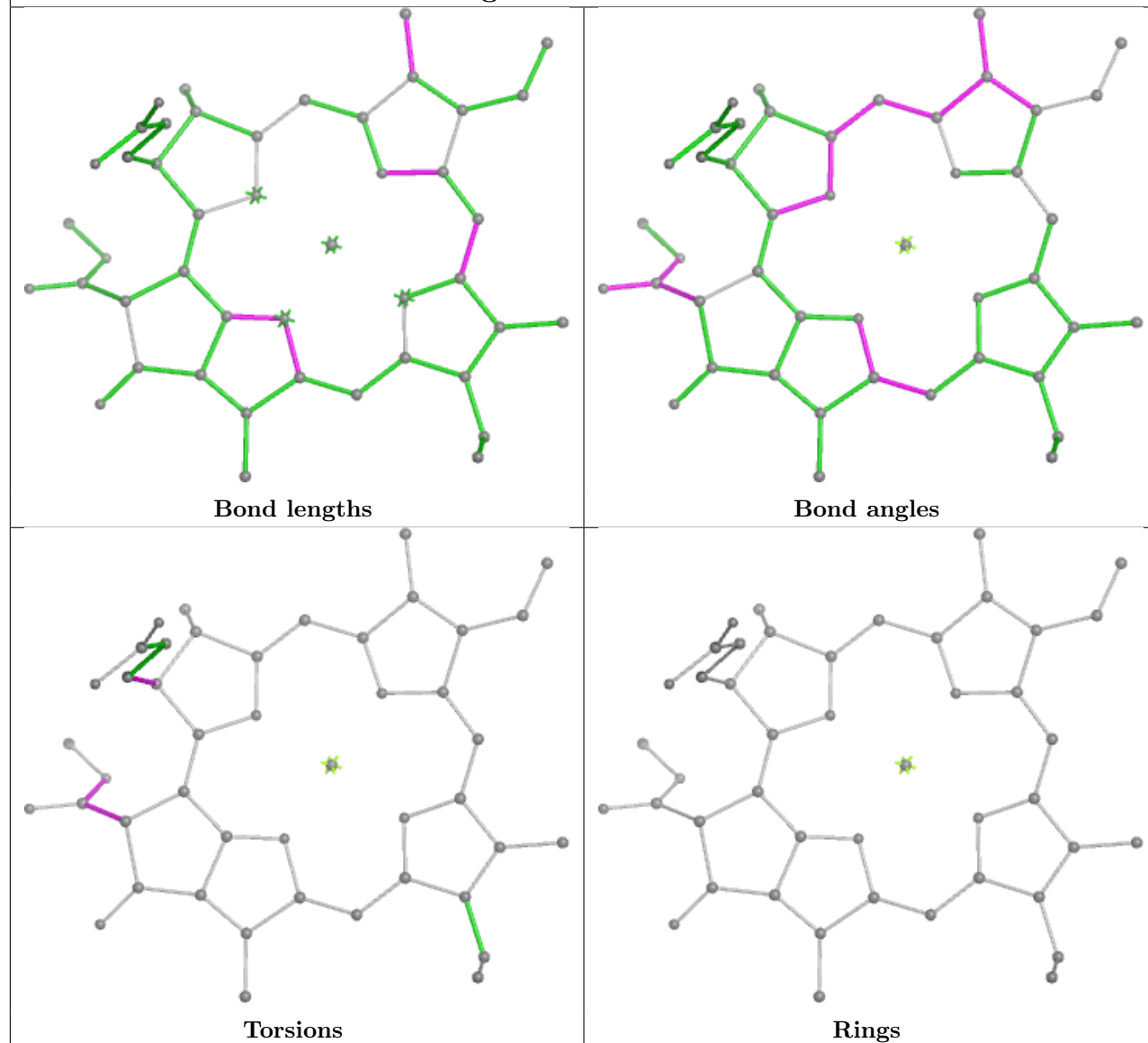




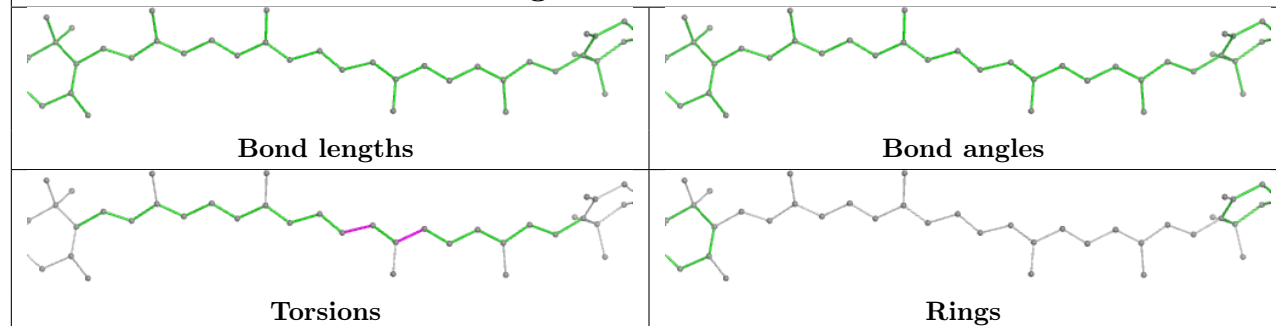
**Ligand CLA a 806****Ligand CLA A 856**



## Ligand CLA b 815

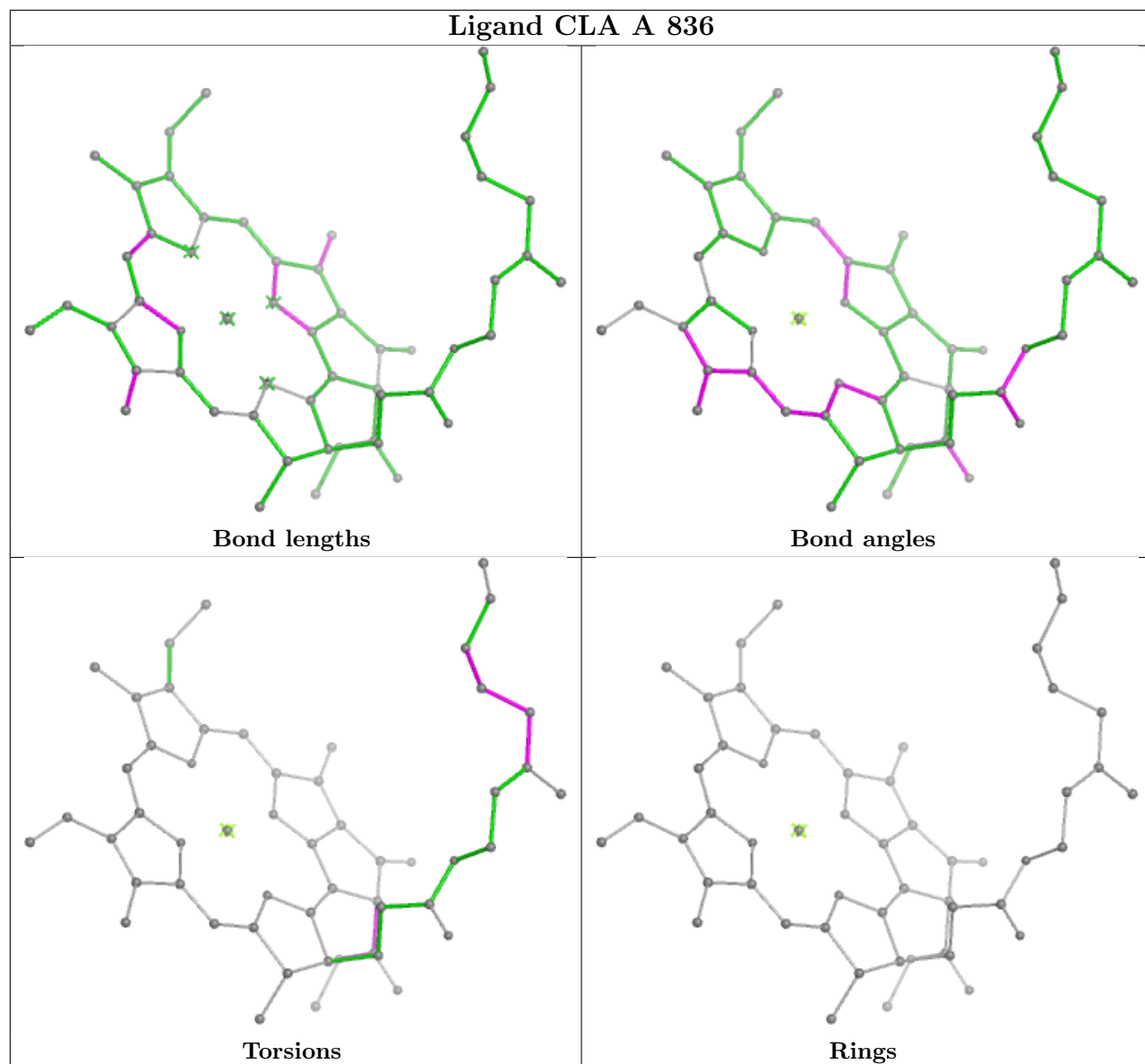


## Ligand BCR N 845

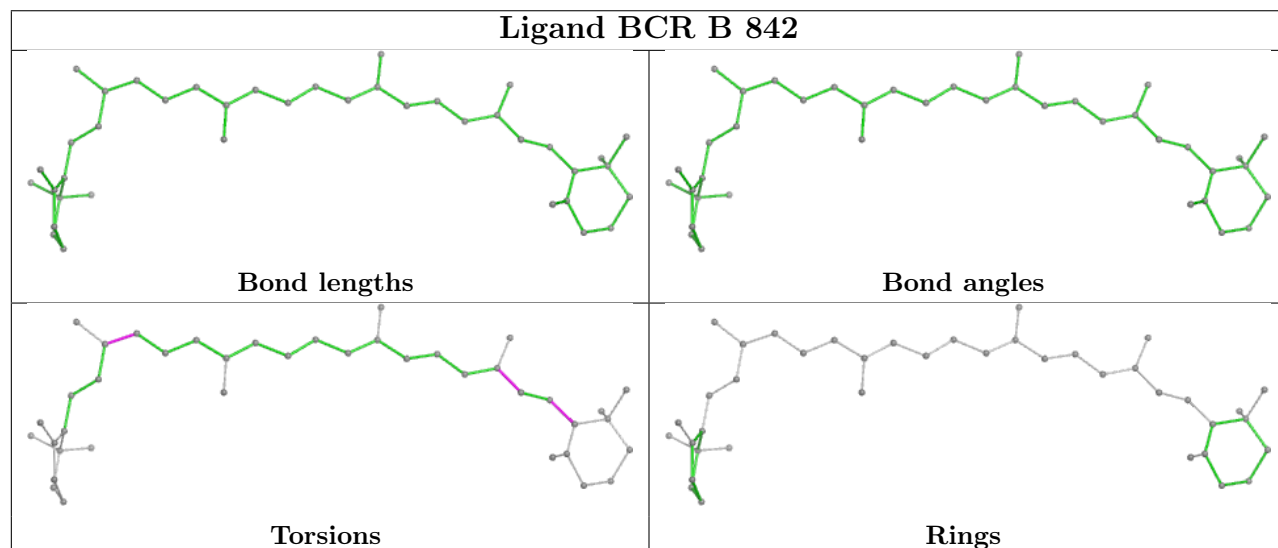




## Ligand CLA A 836

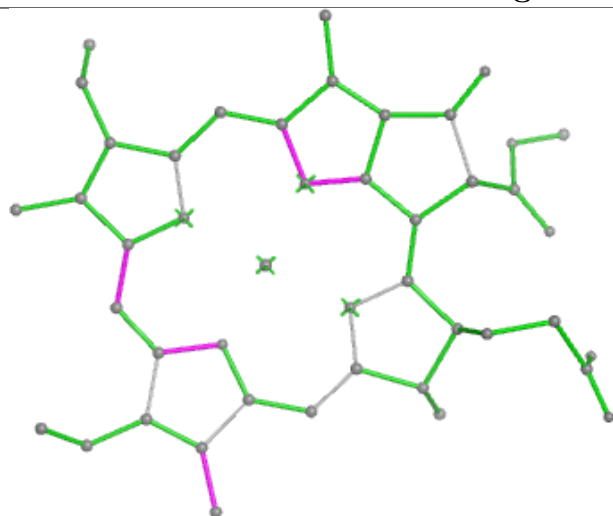


## Ligand BCR B 842

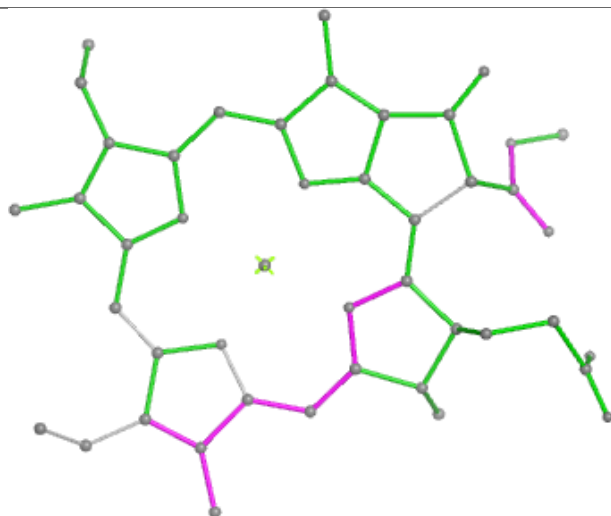




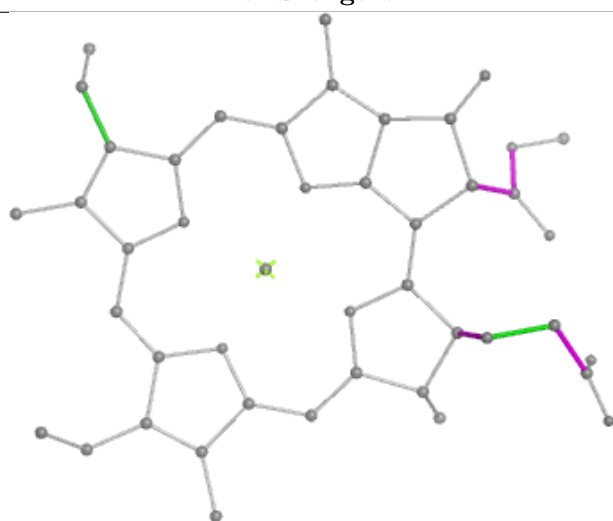
## Ligand CLA O 836



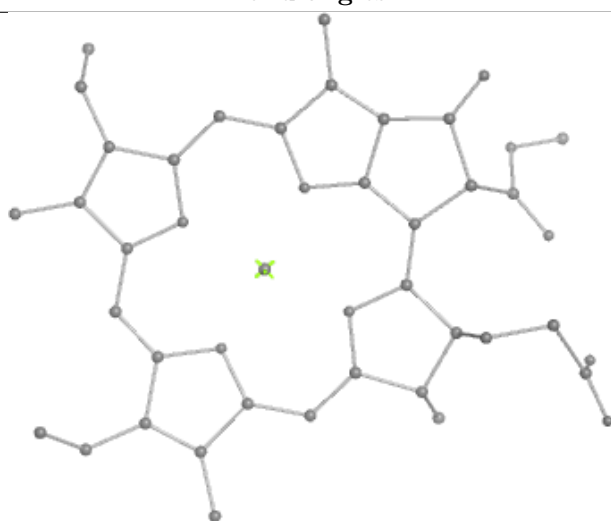
Bond lengths



Bond angles

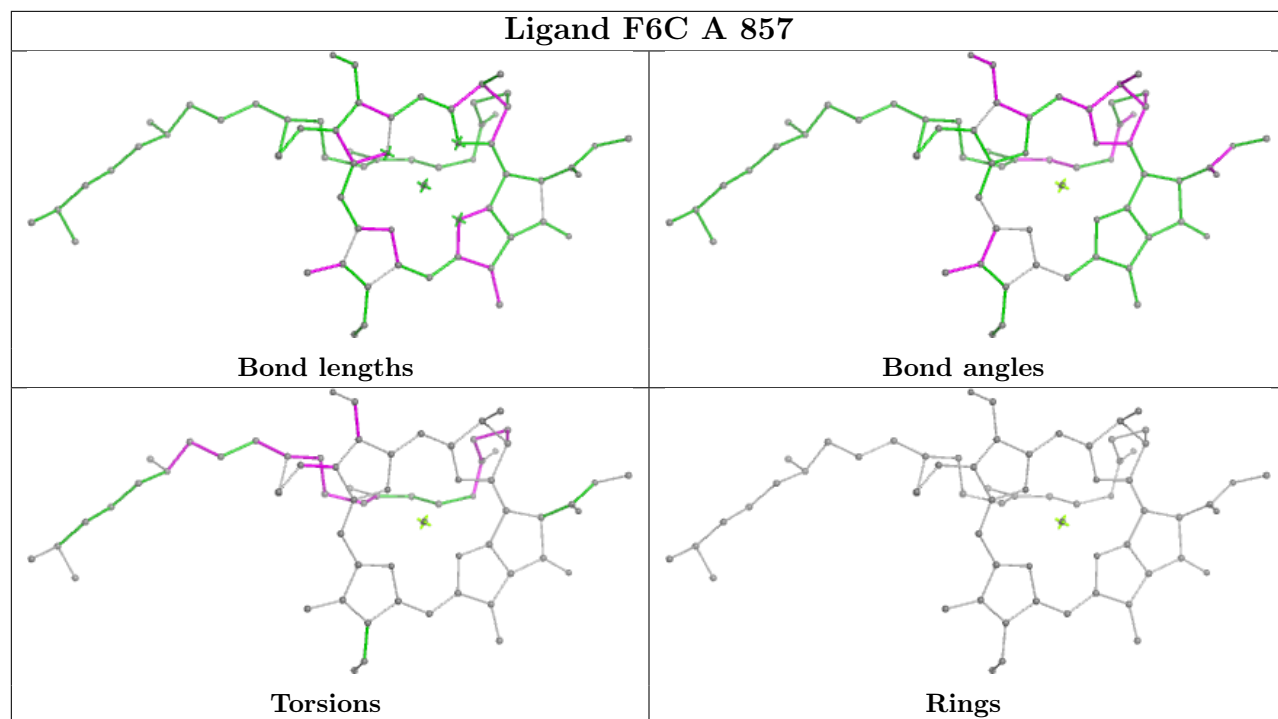


Torsions

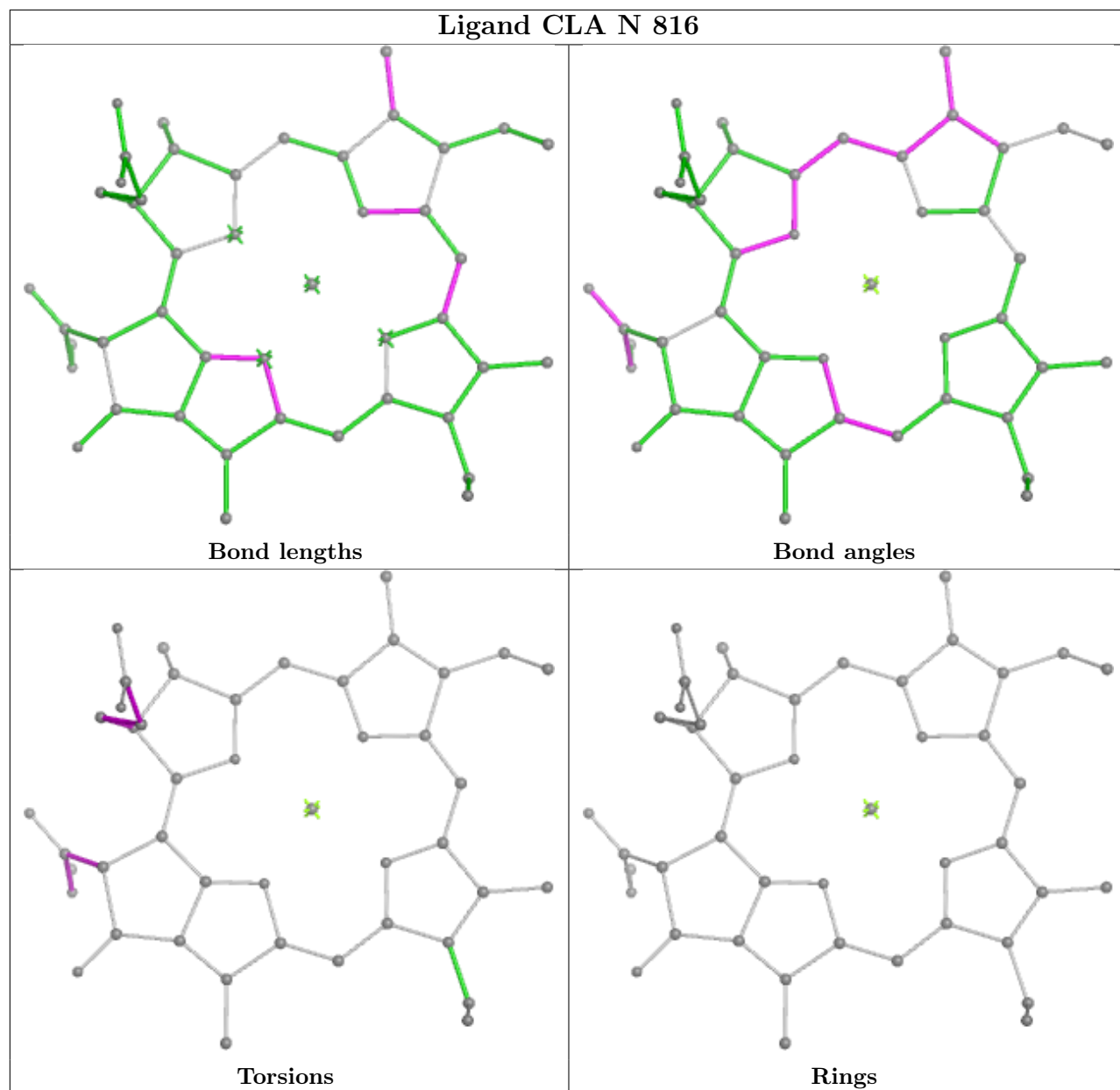


Rings



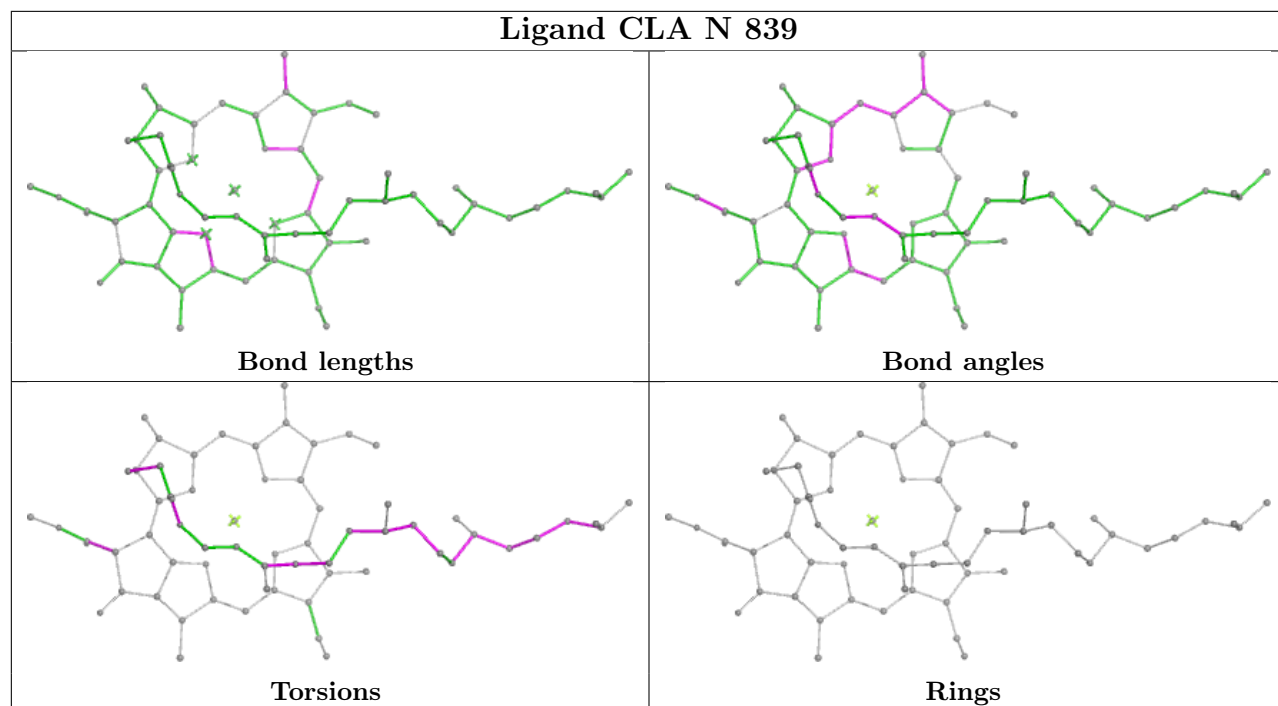




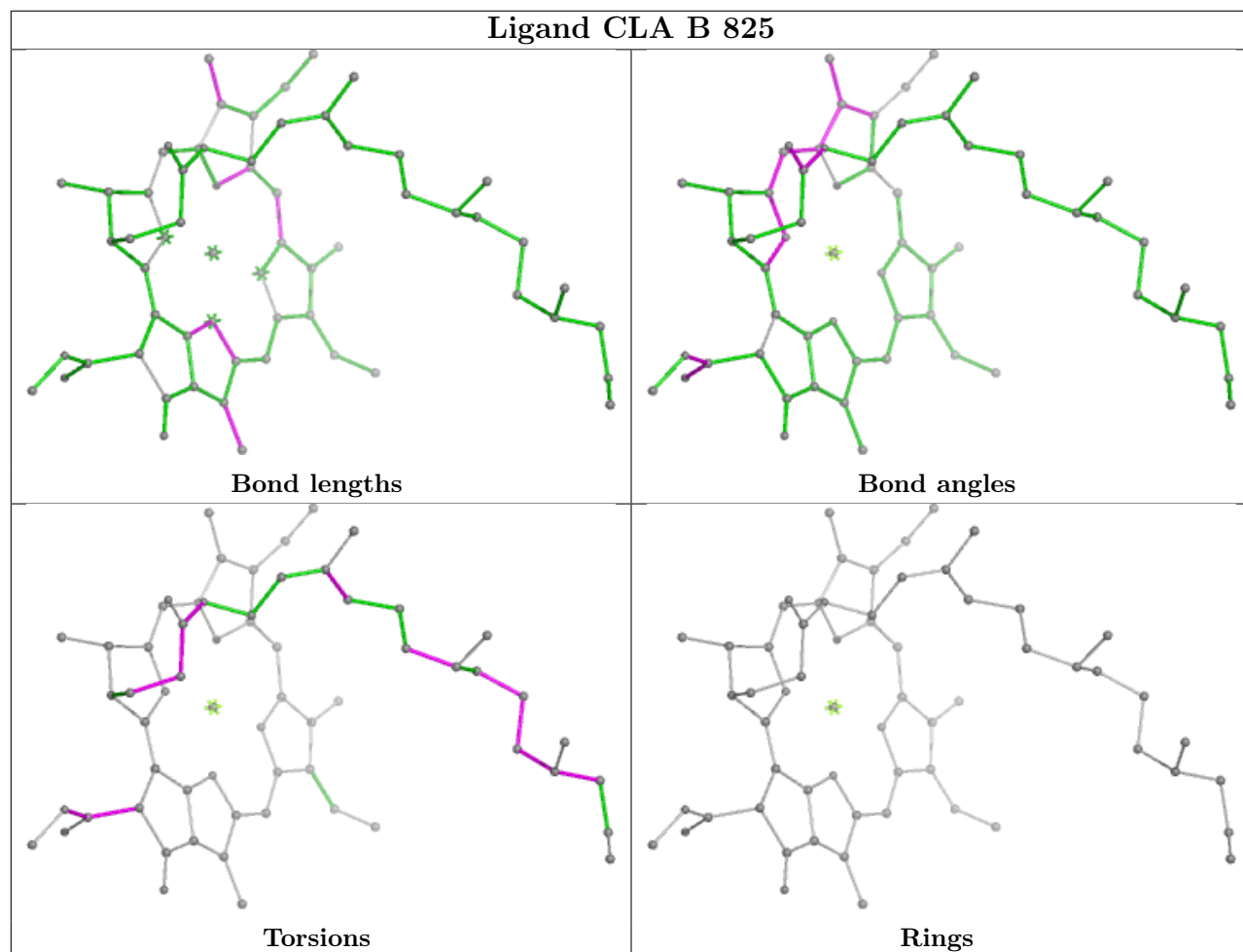




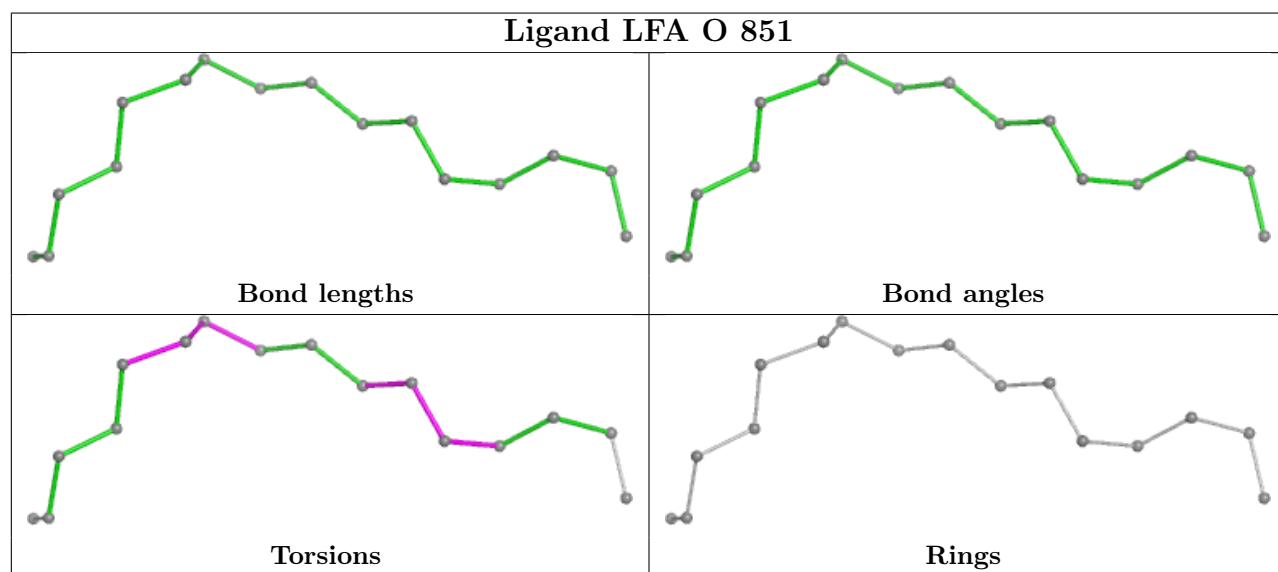
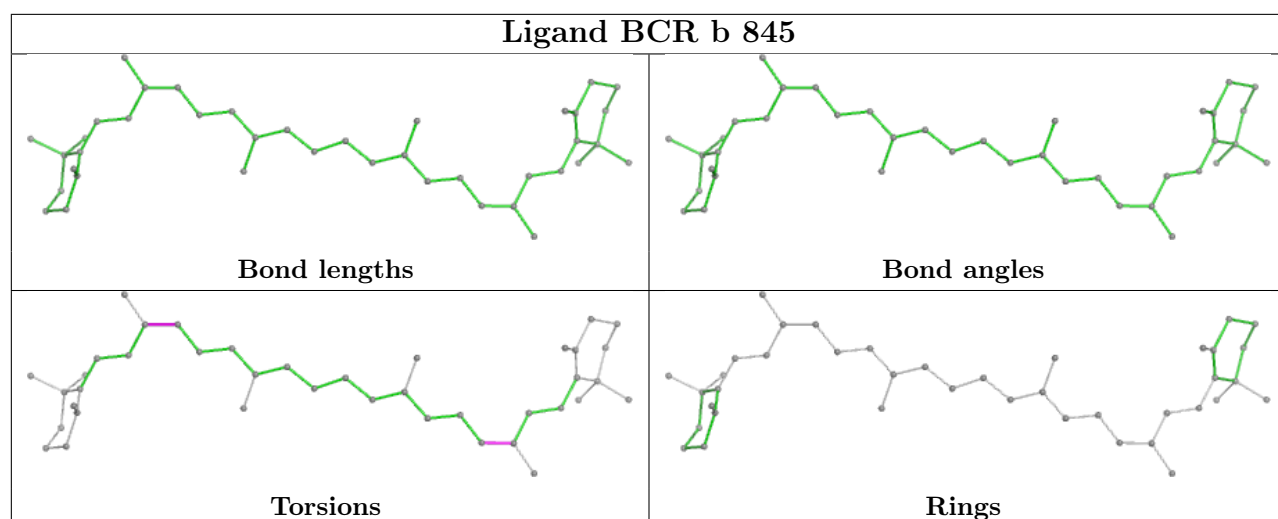
## Ligand CLA N 839



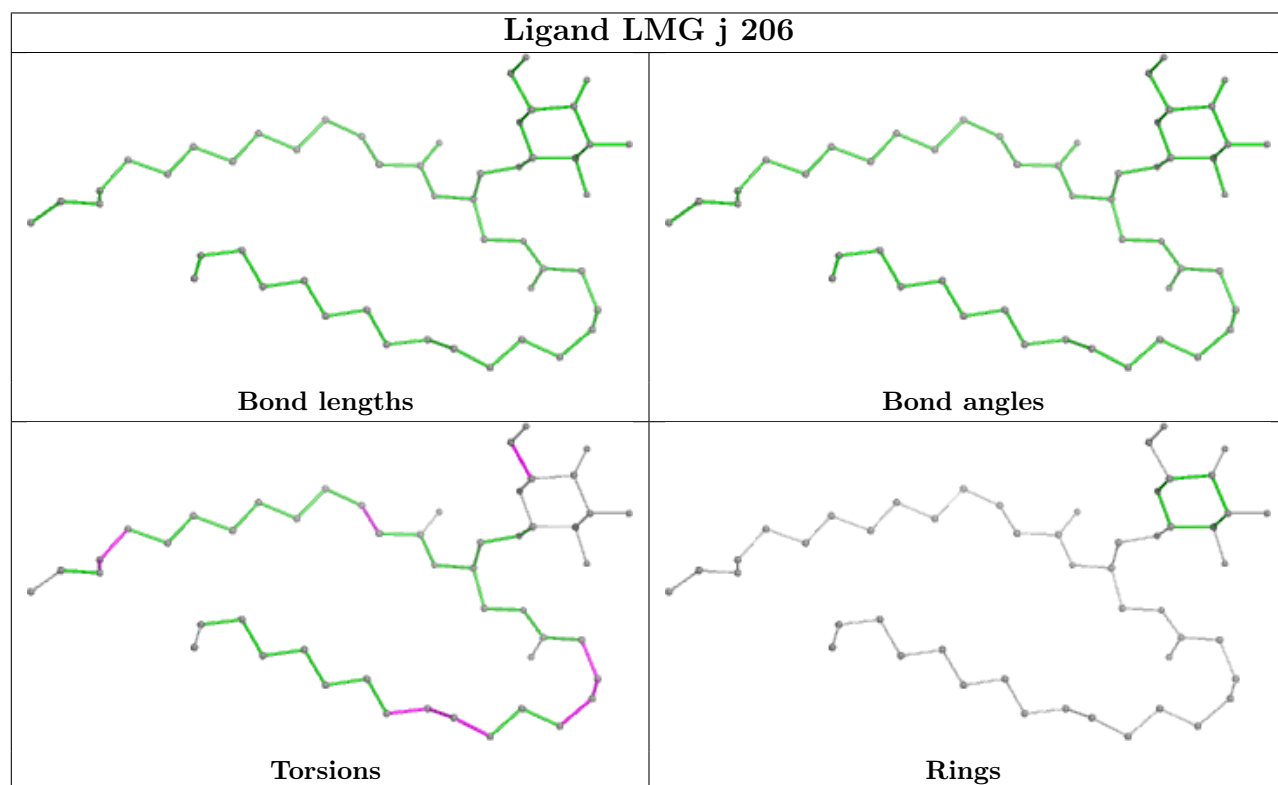
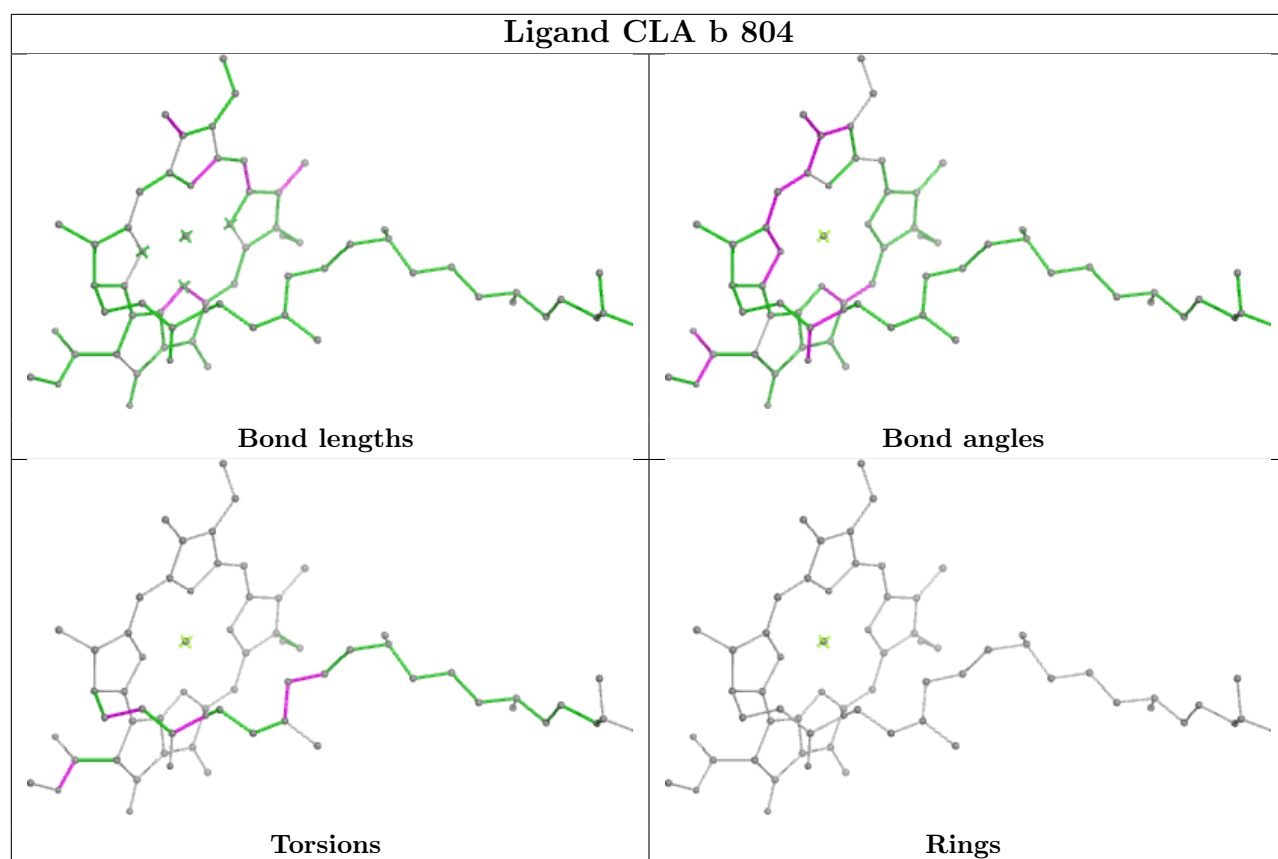
## Ligand CLA B 825





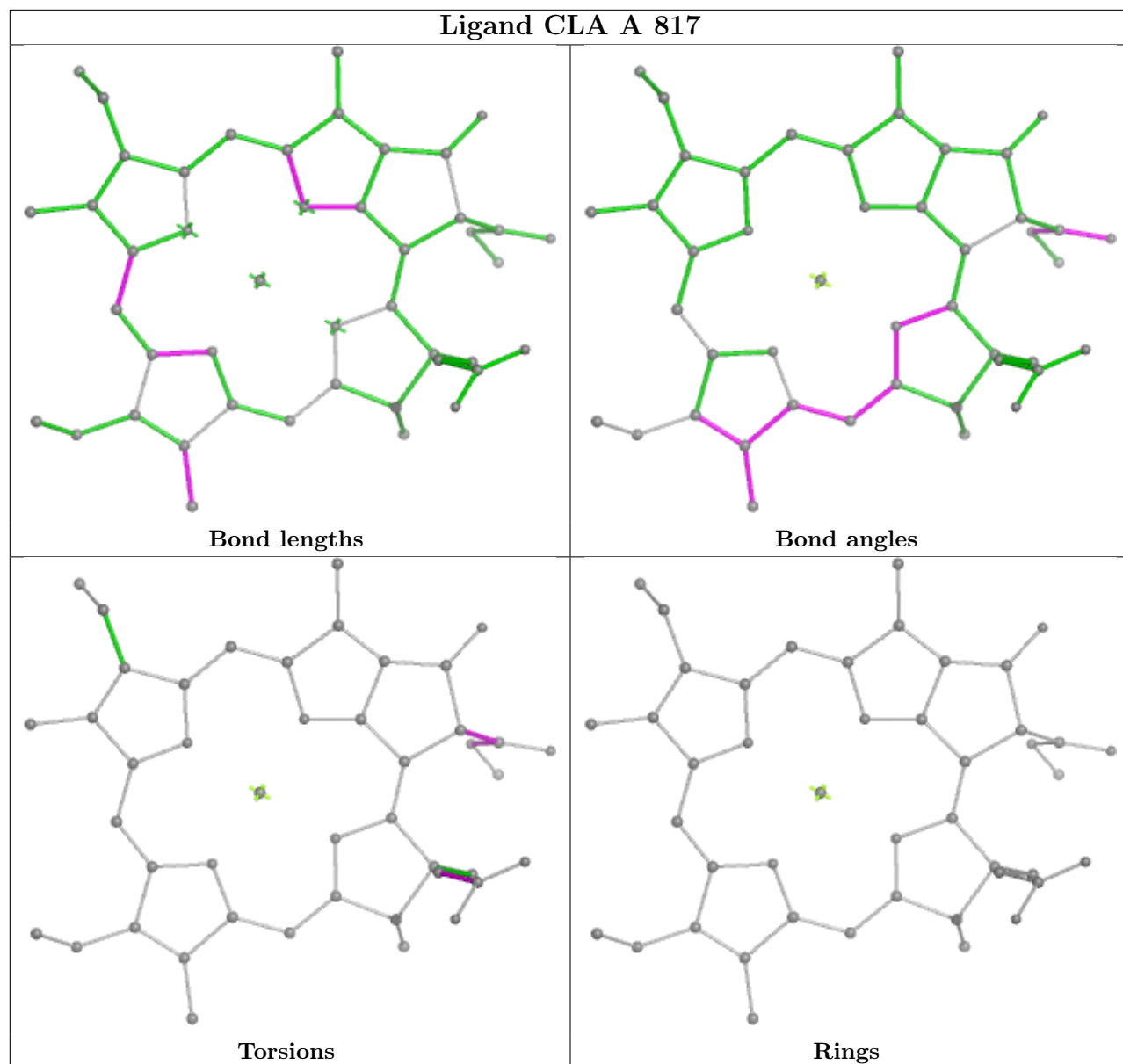






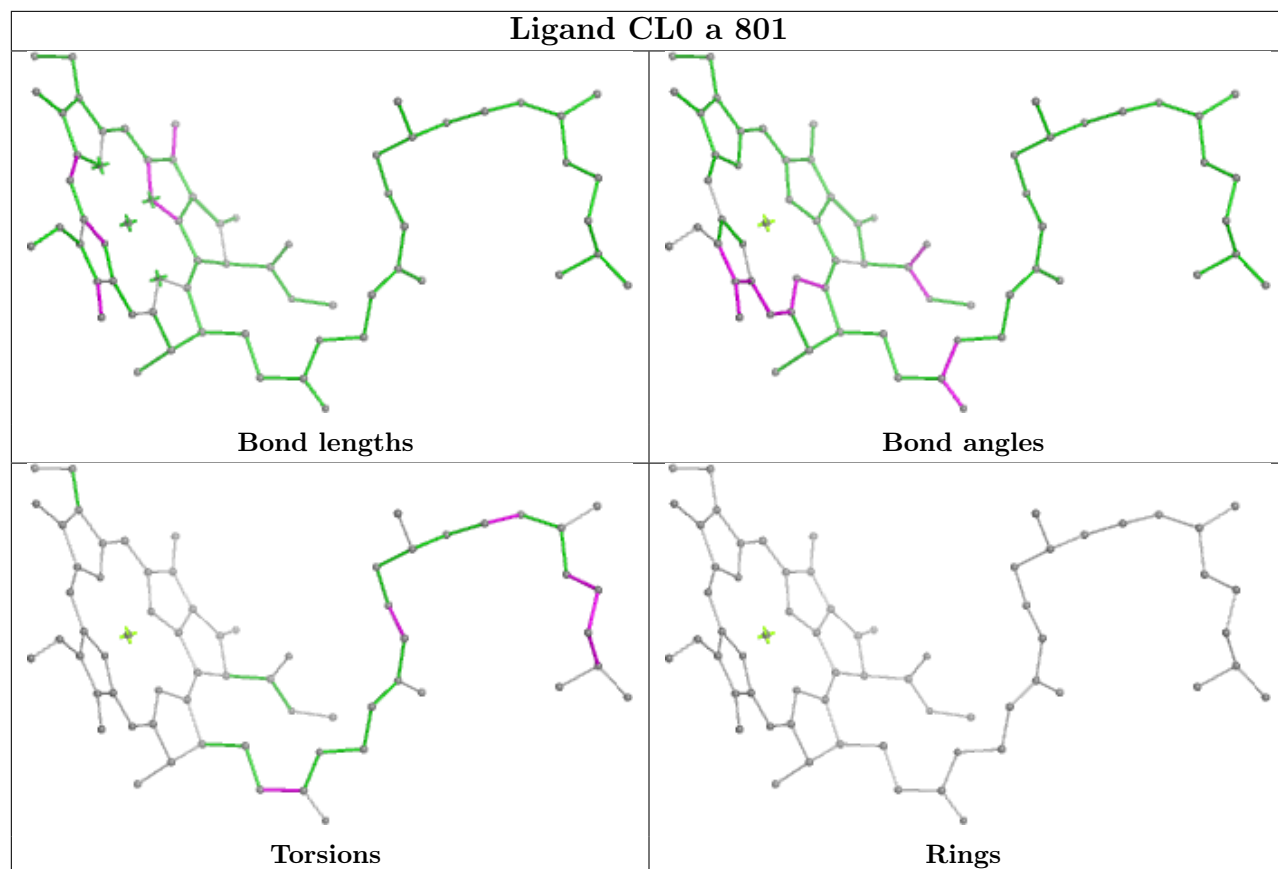


## Ligand CLA A 817

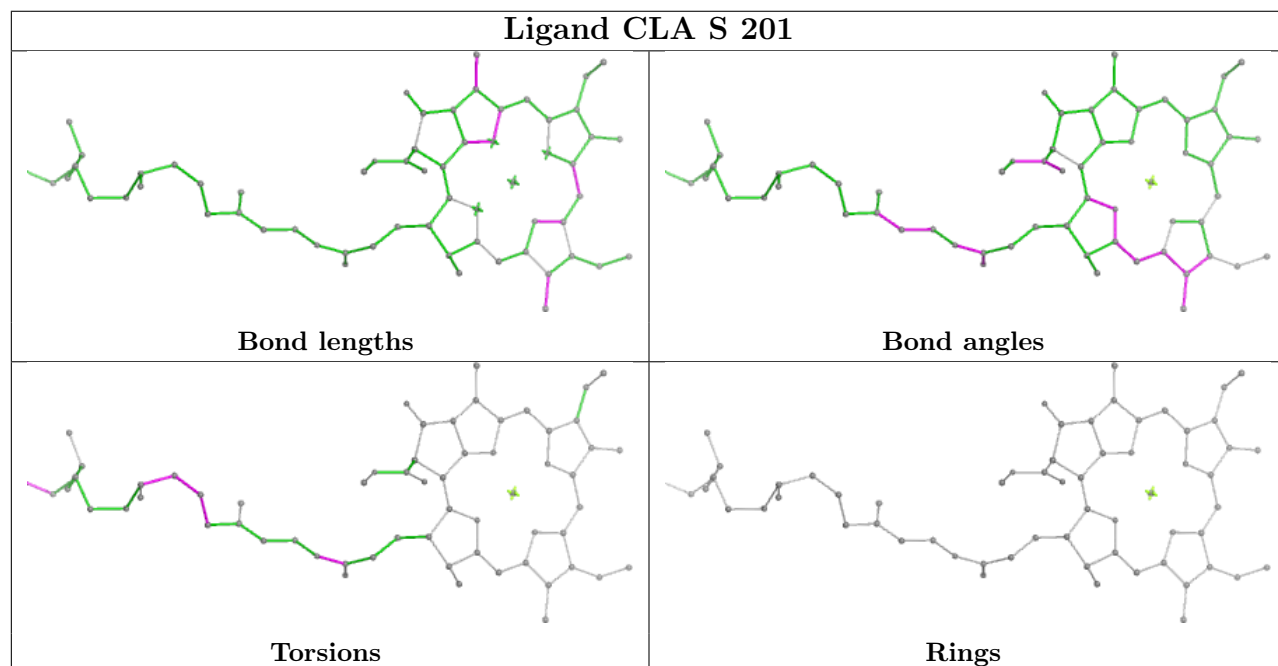




## Ligand CL0 a 801

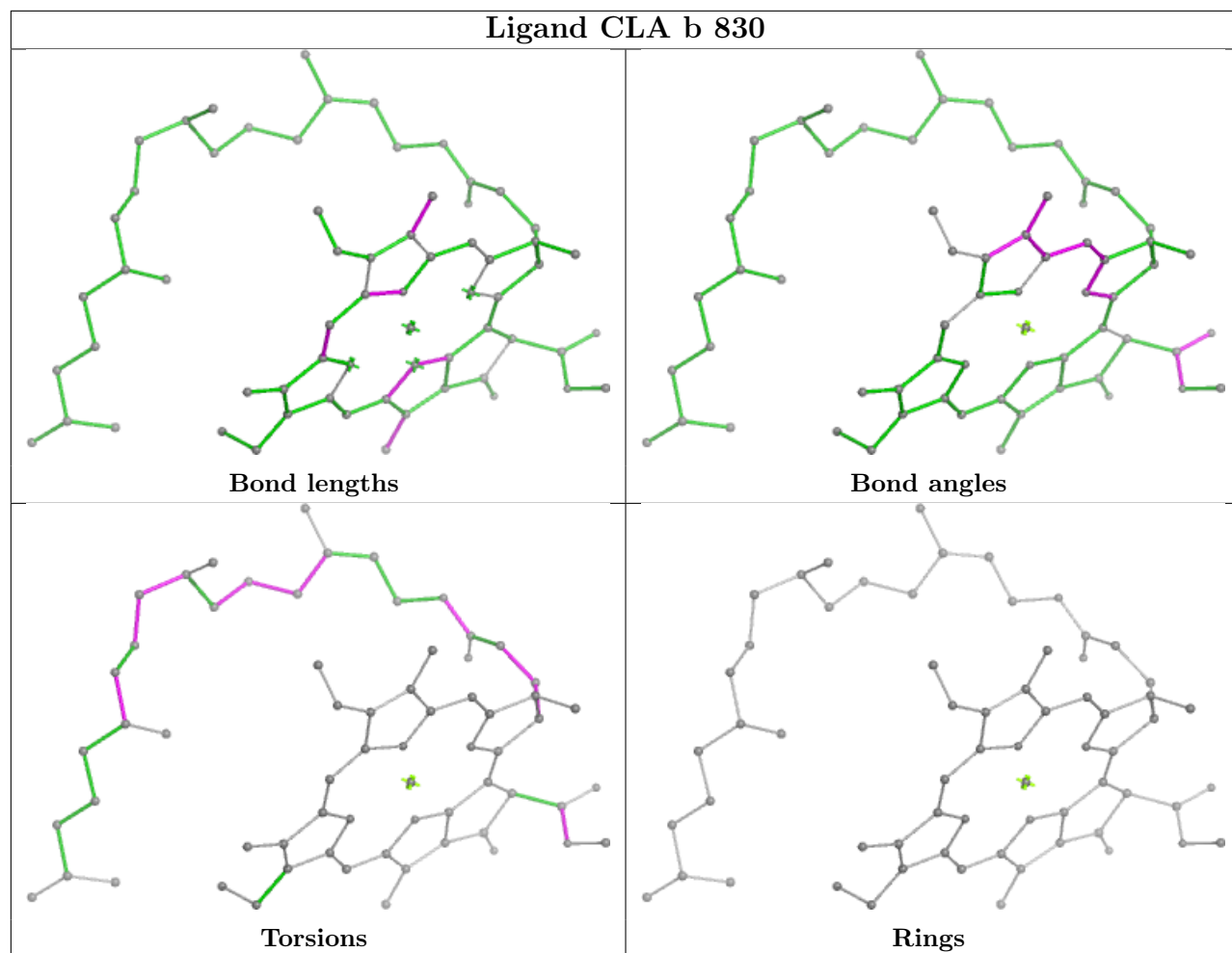


## Ligand CLA S 201

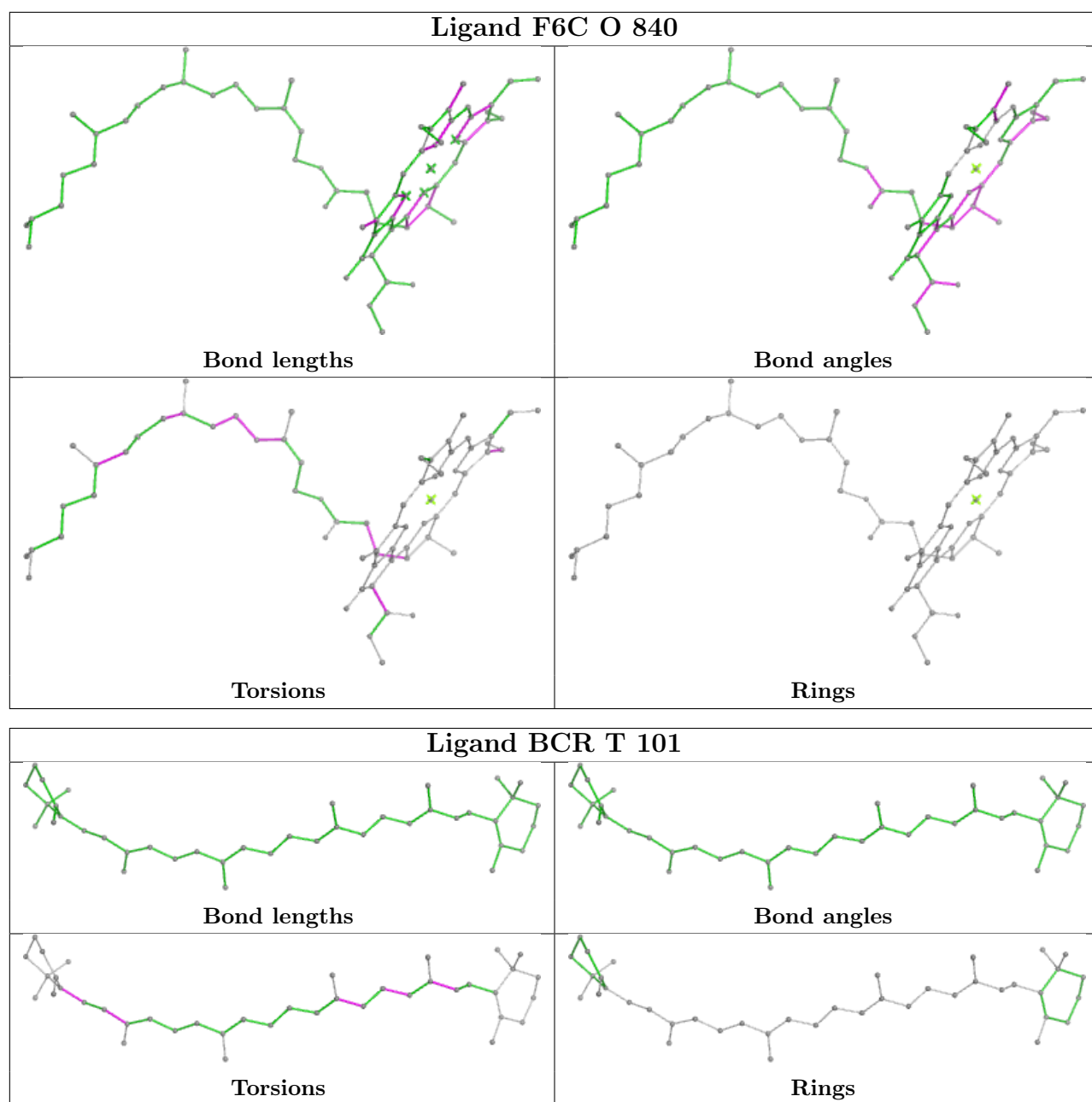




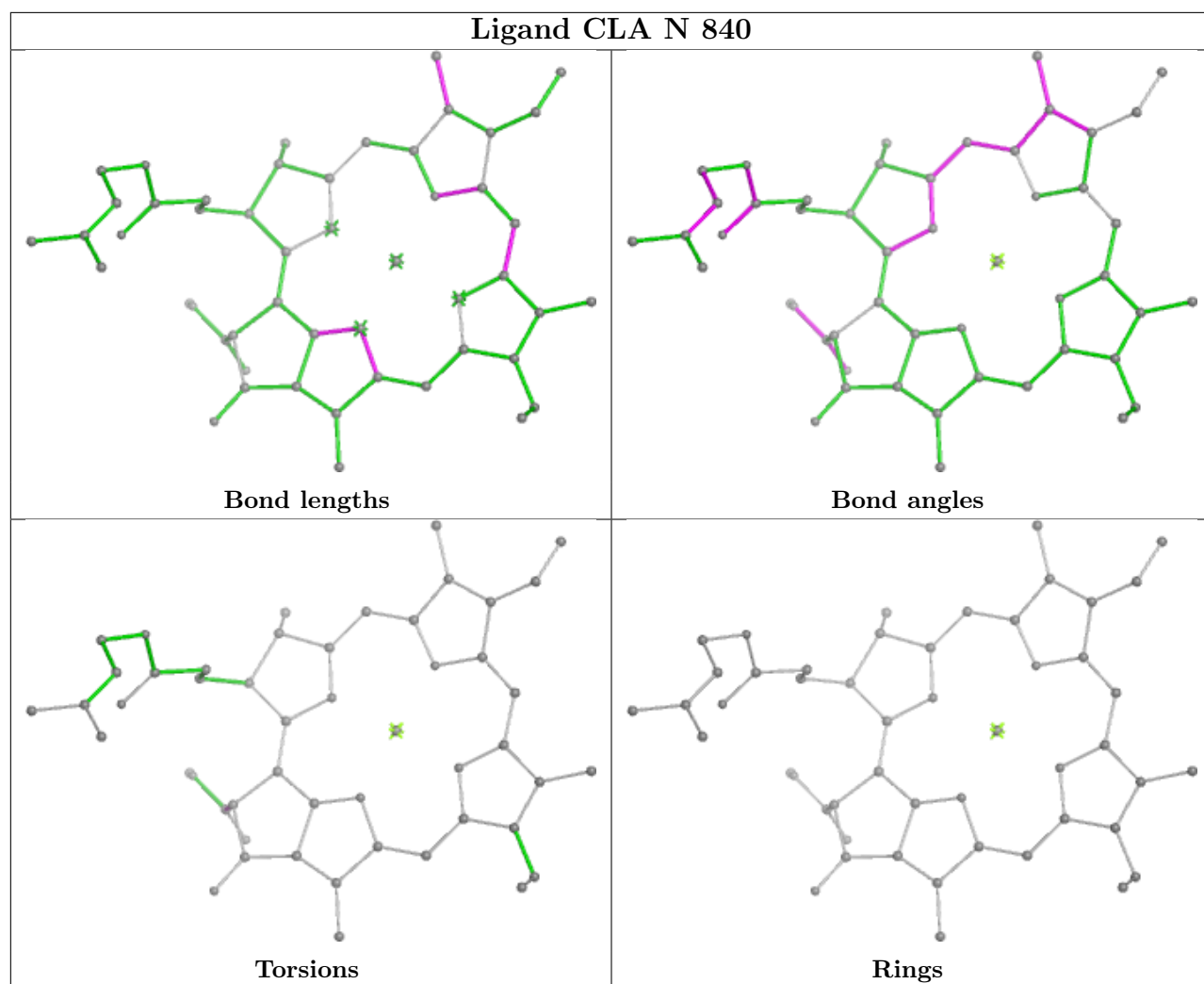
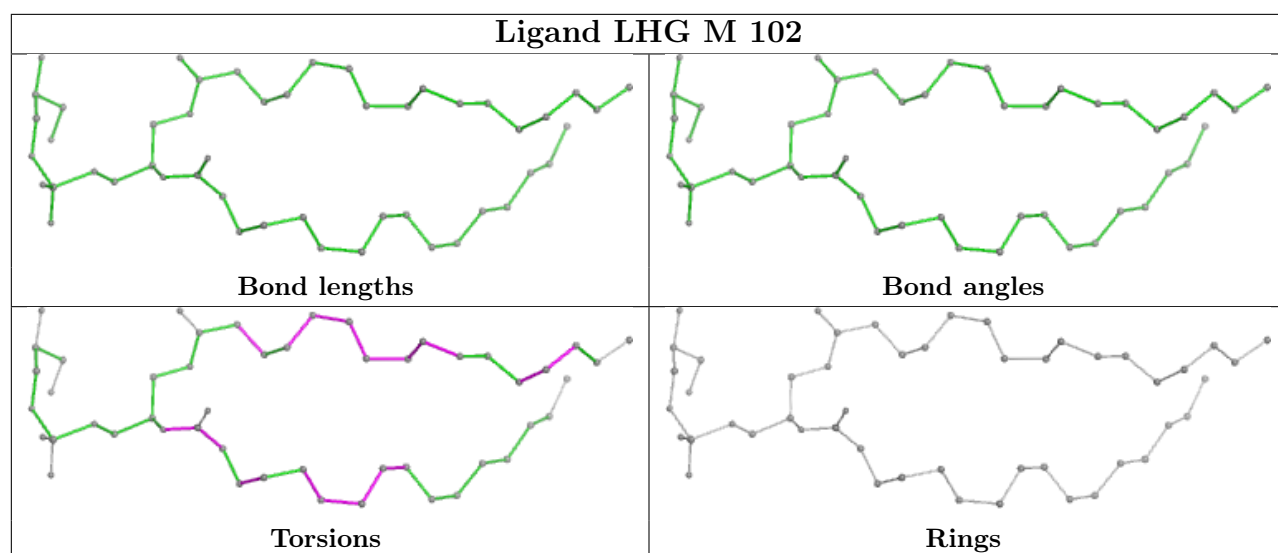
## Ligand CLA b 830





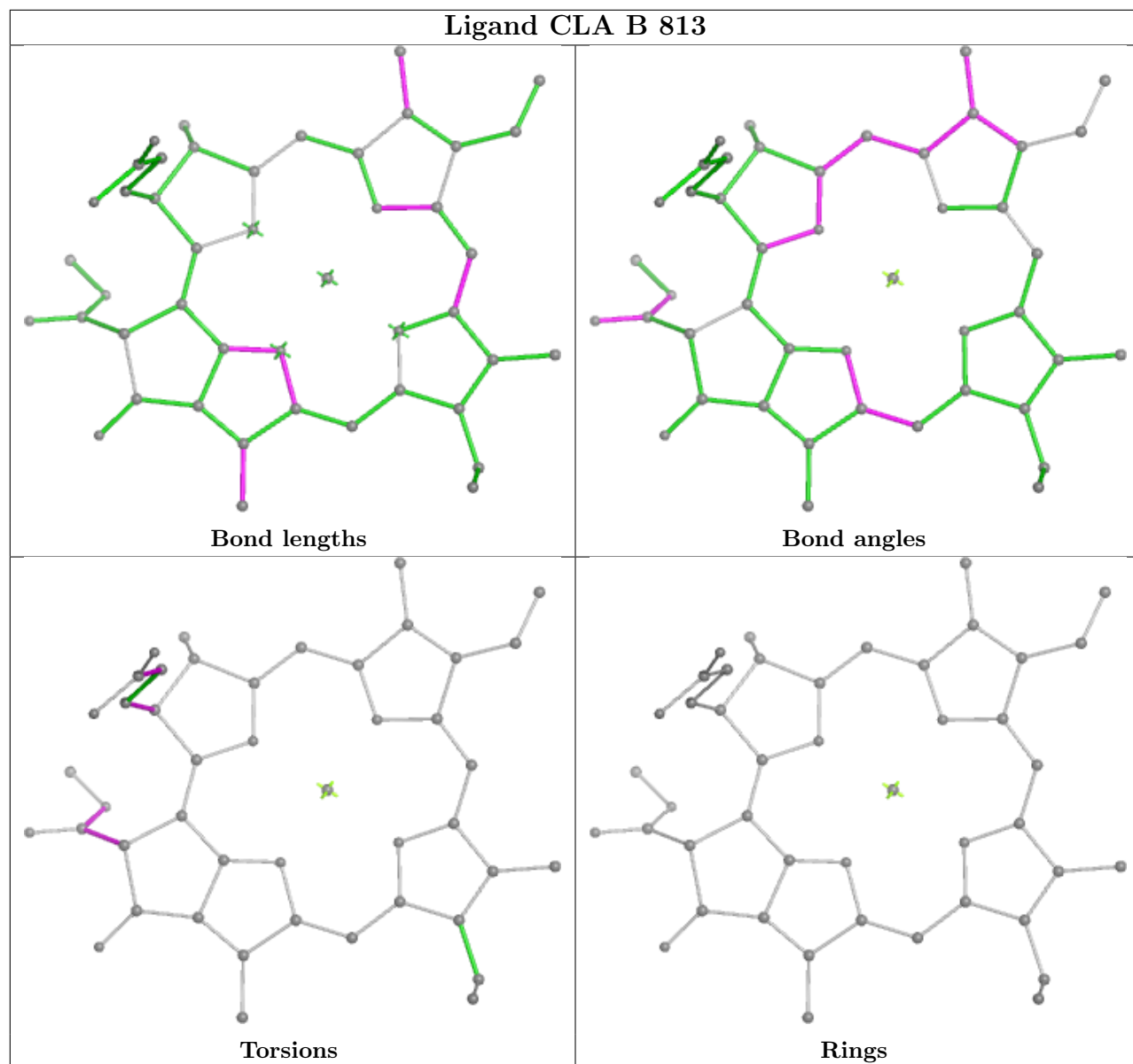




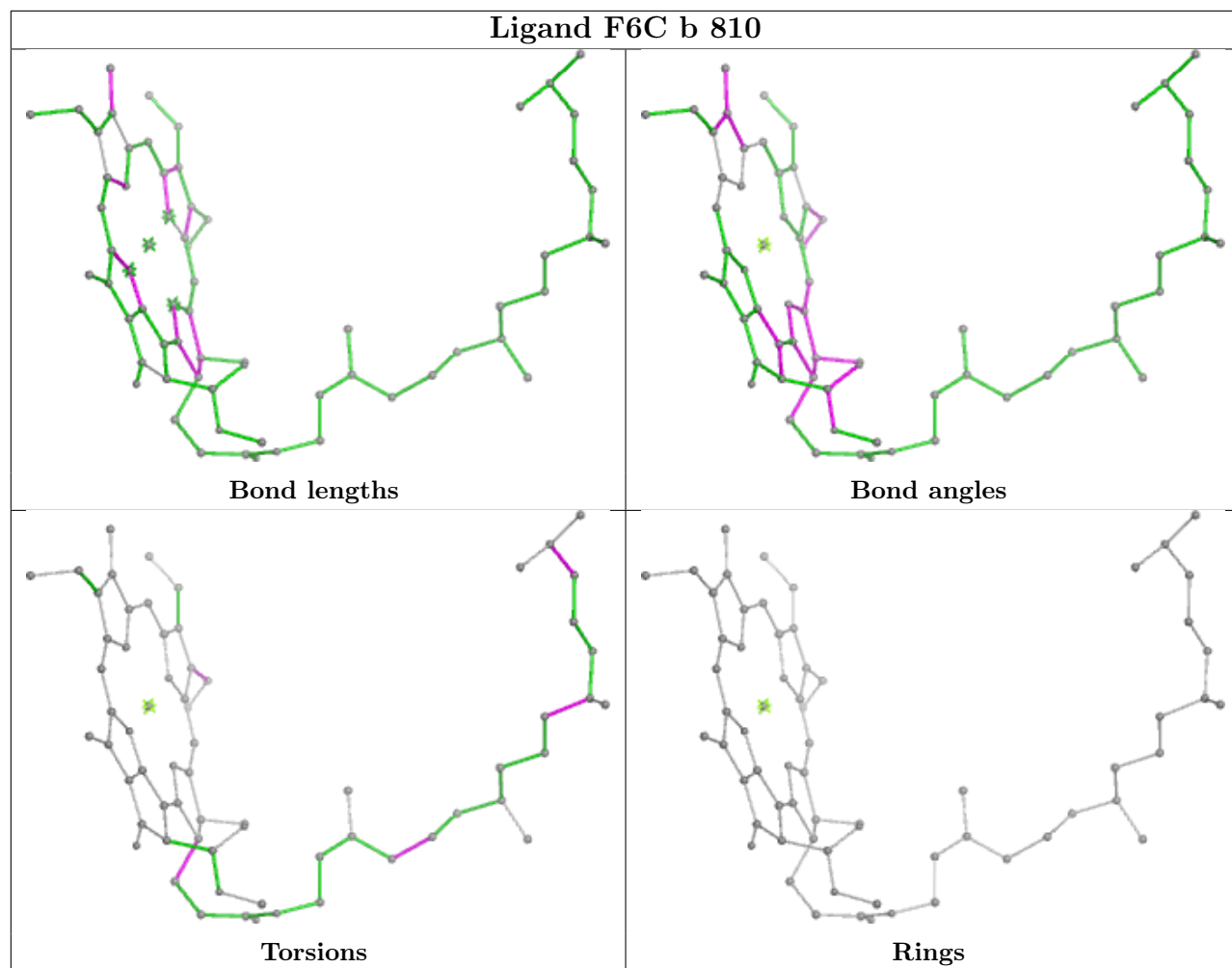




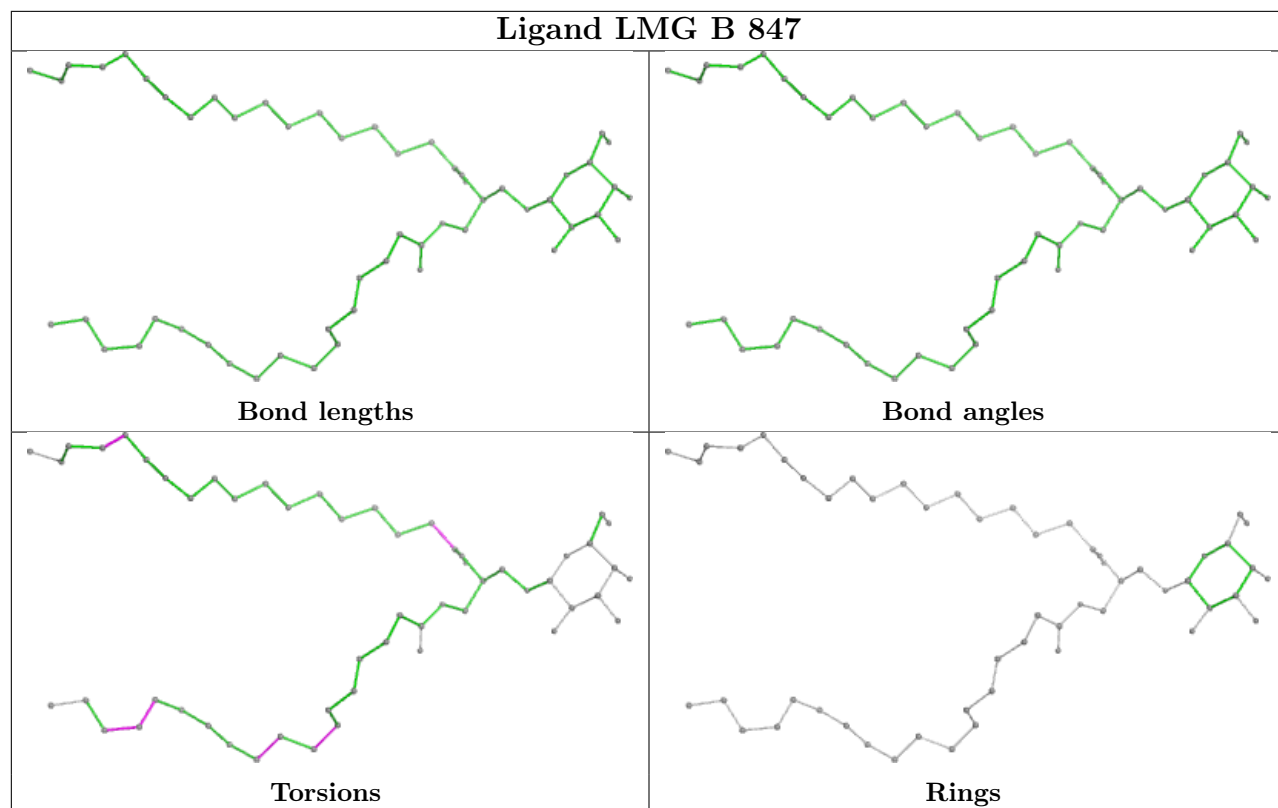
## Ligand CLA B 813





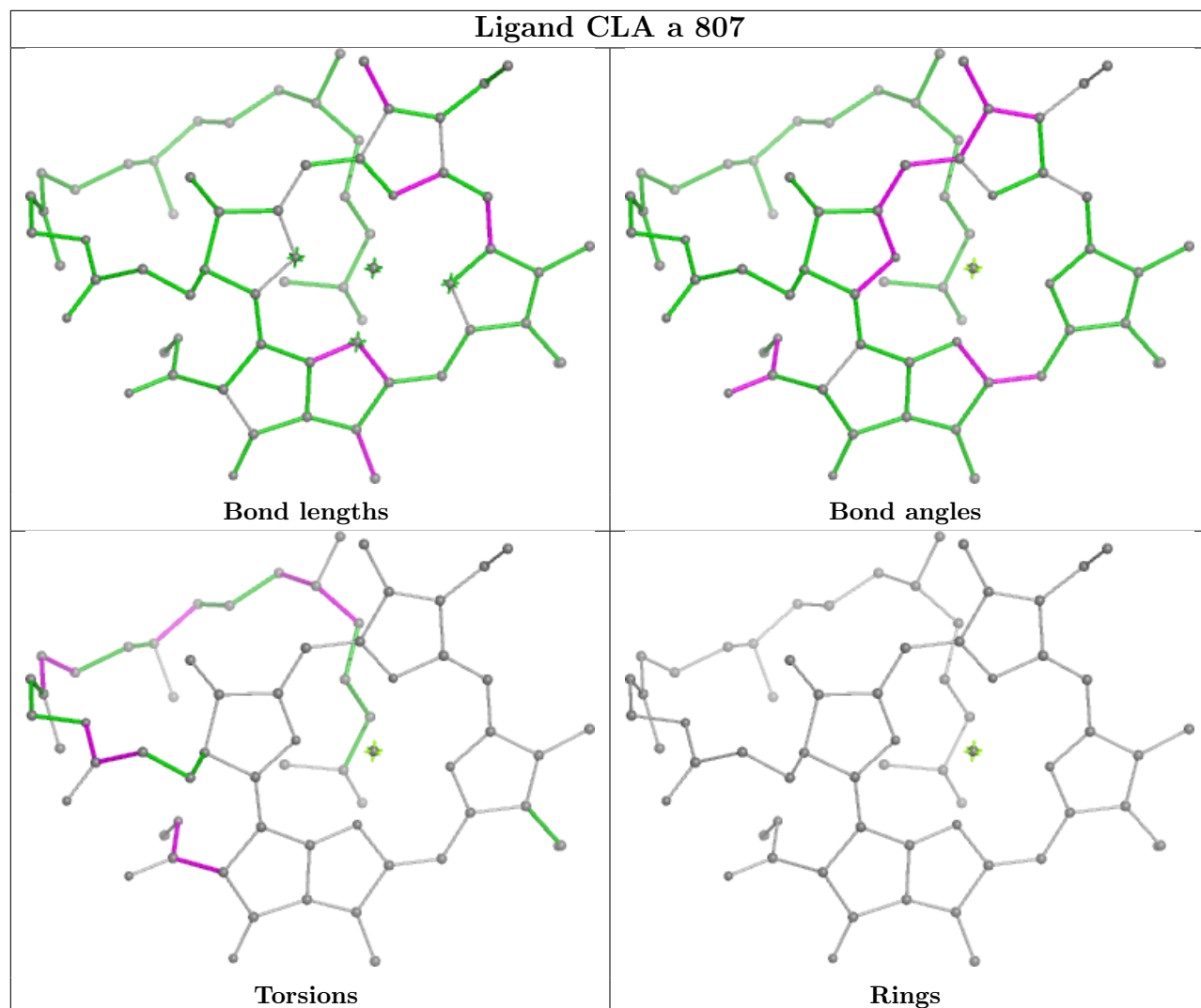




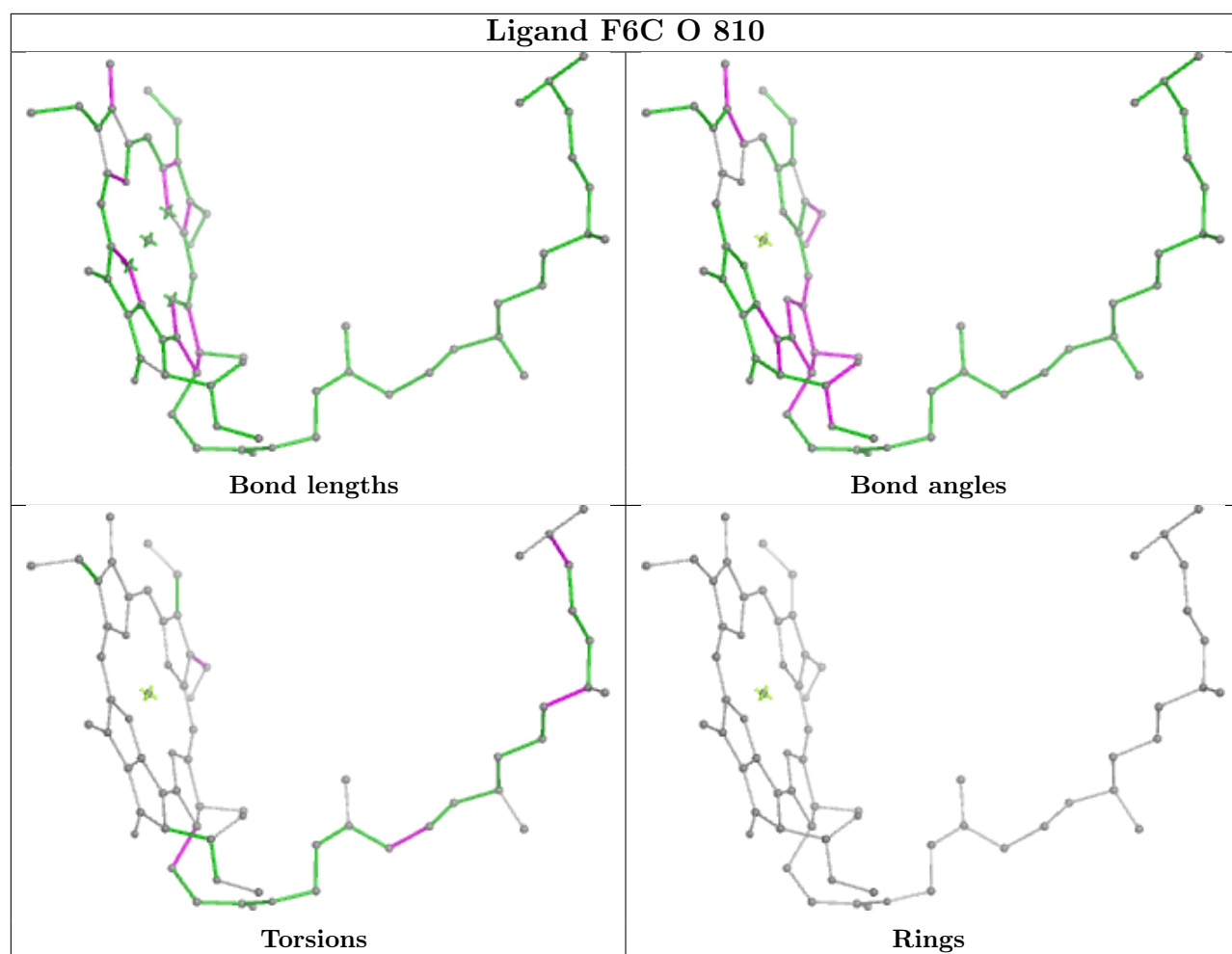




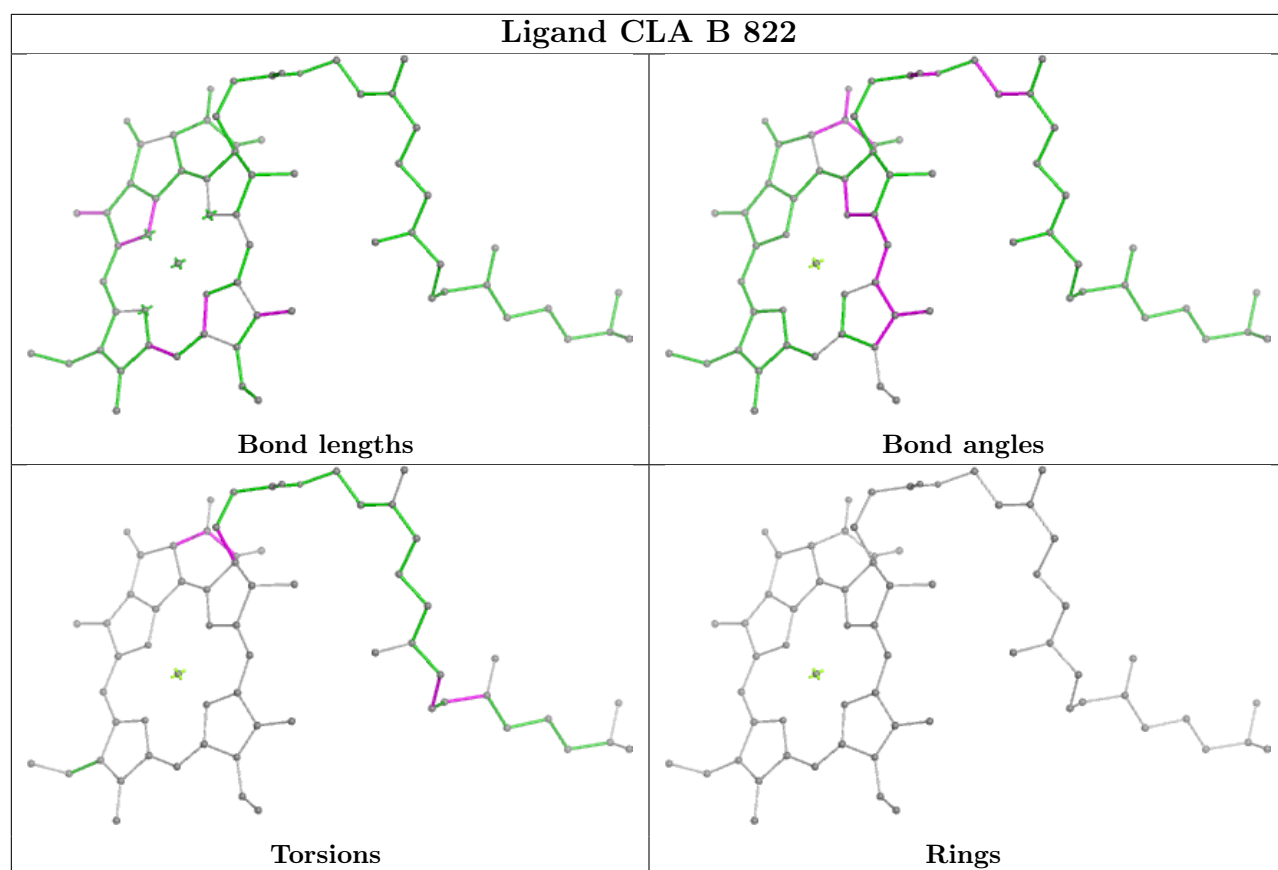
## Ligand CLA a 807





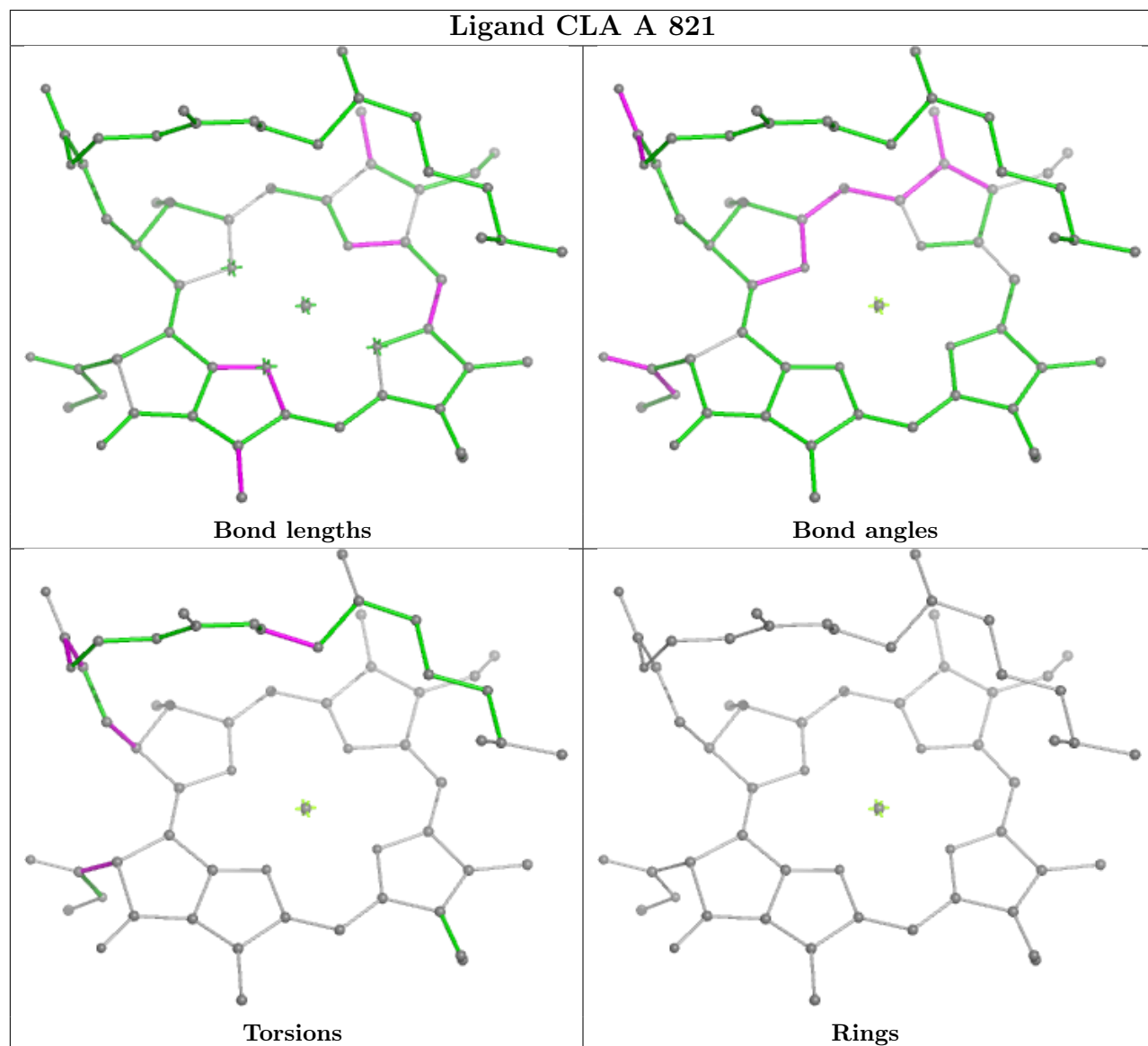




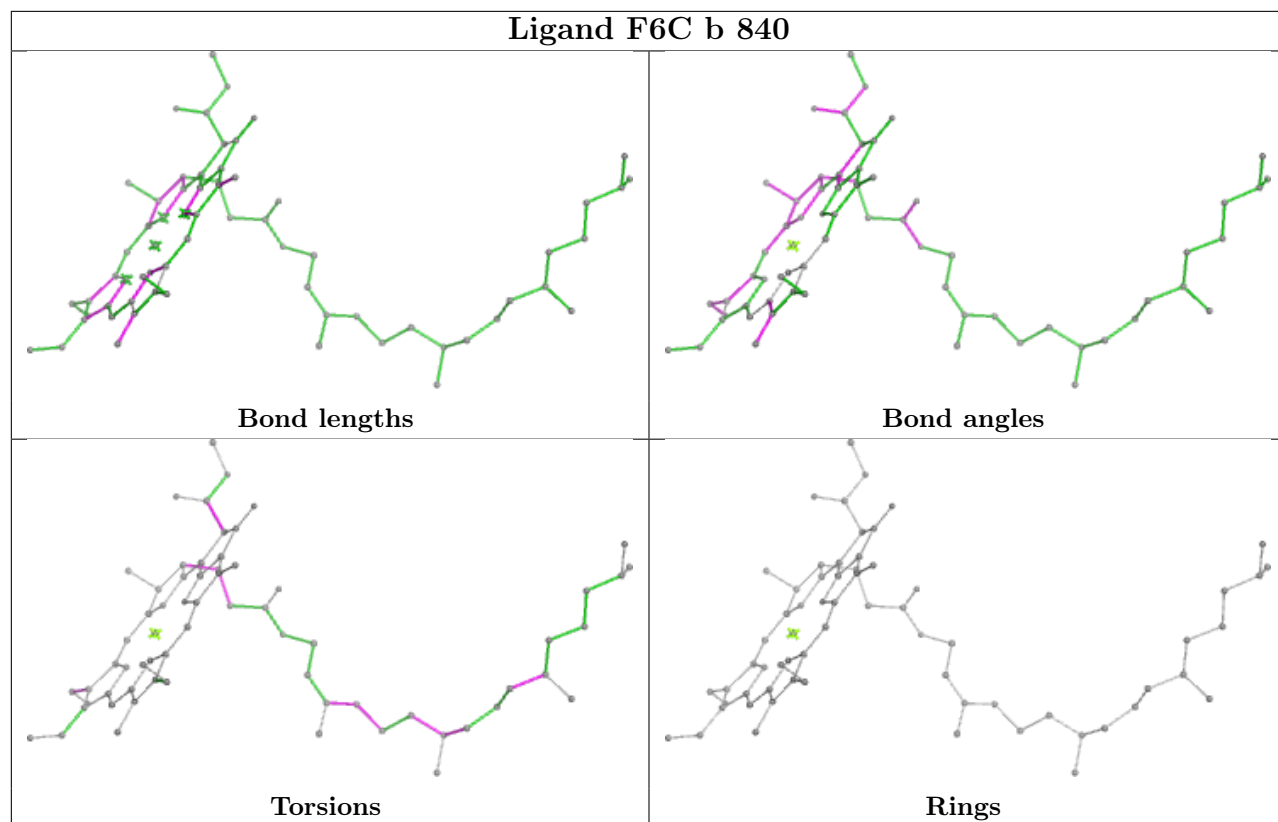
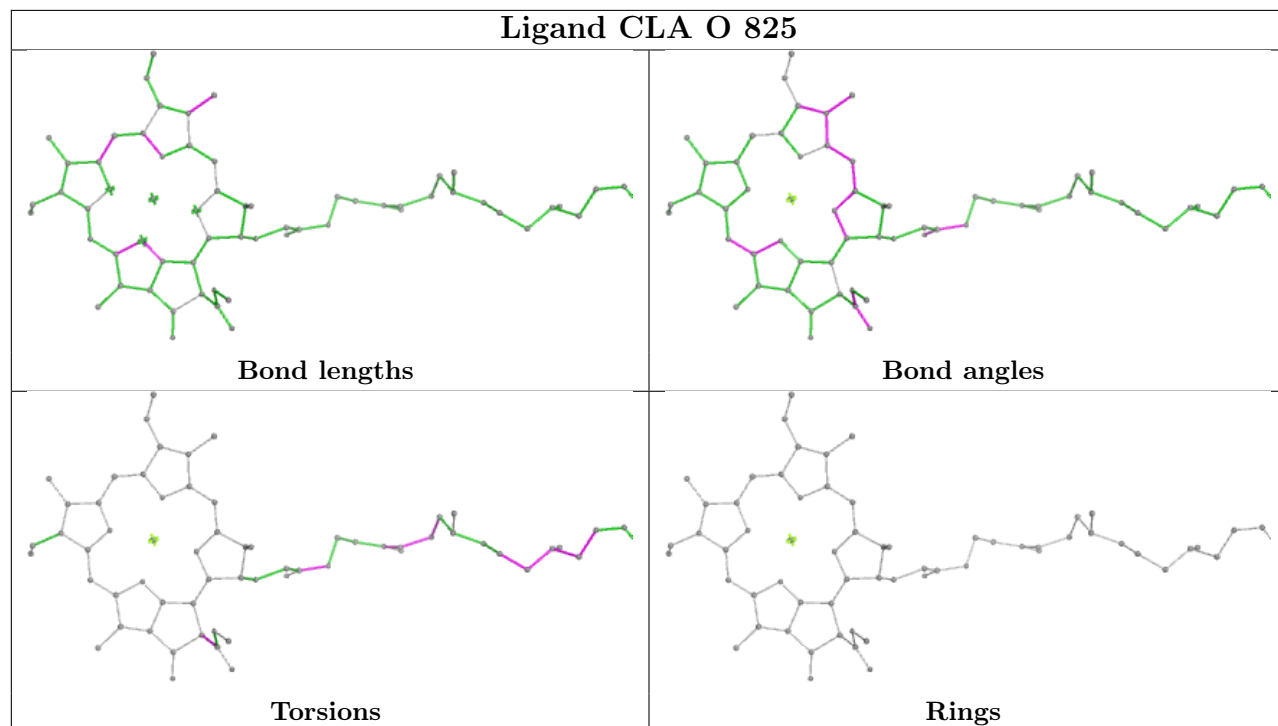




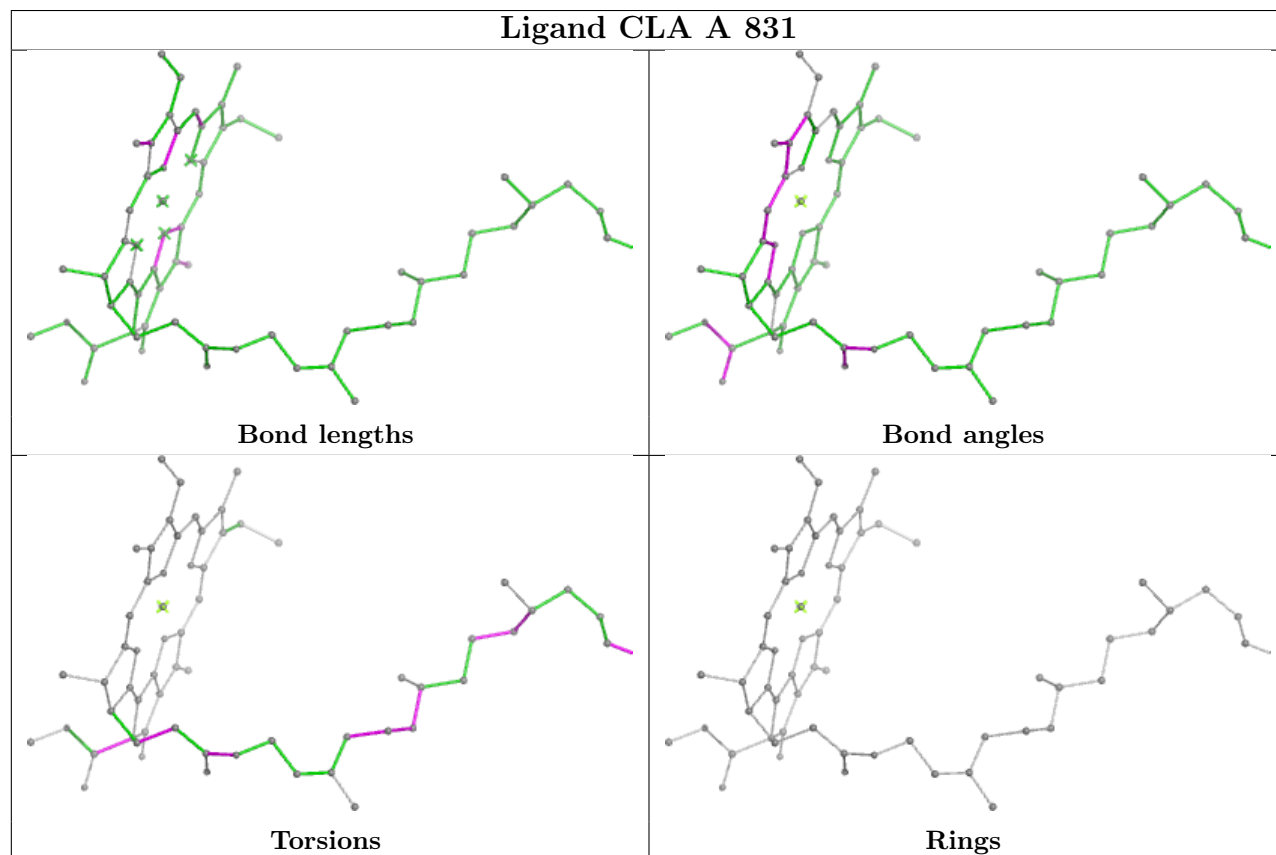
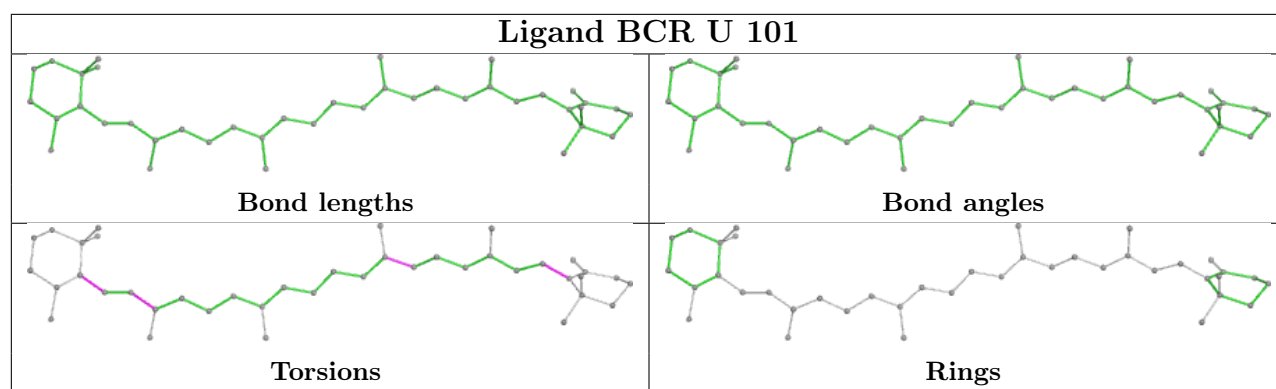
## Ligand CLA A 821



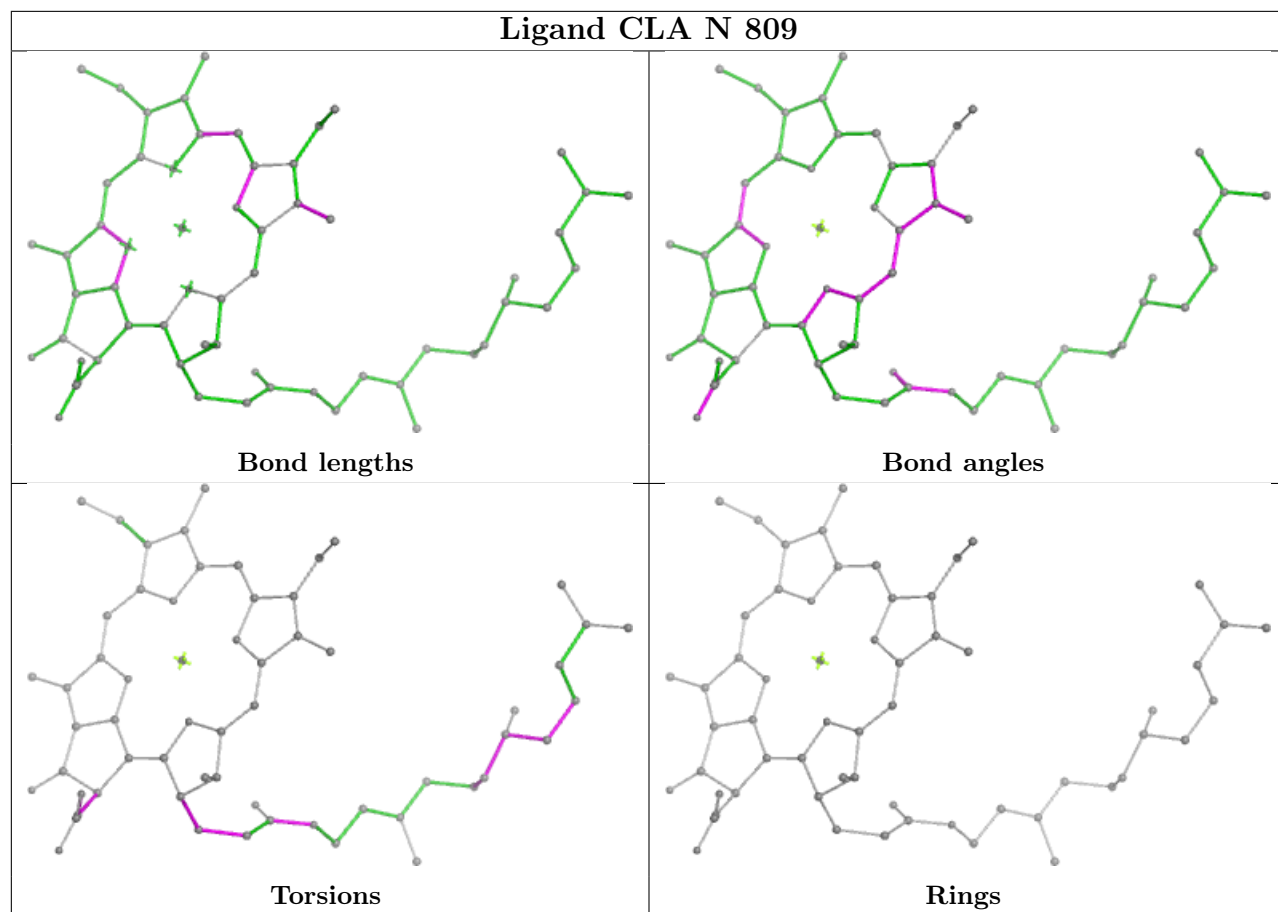


**Ligand F6C b 840****Ligand CLA O 825**

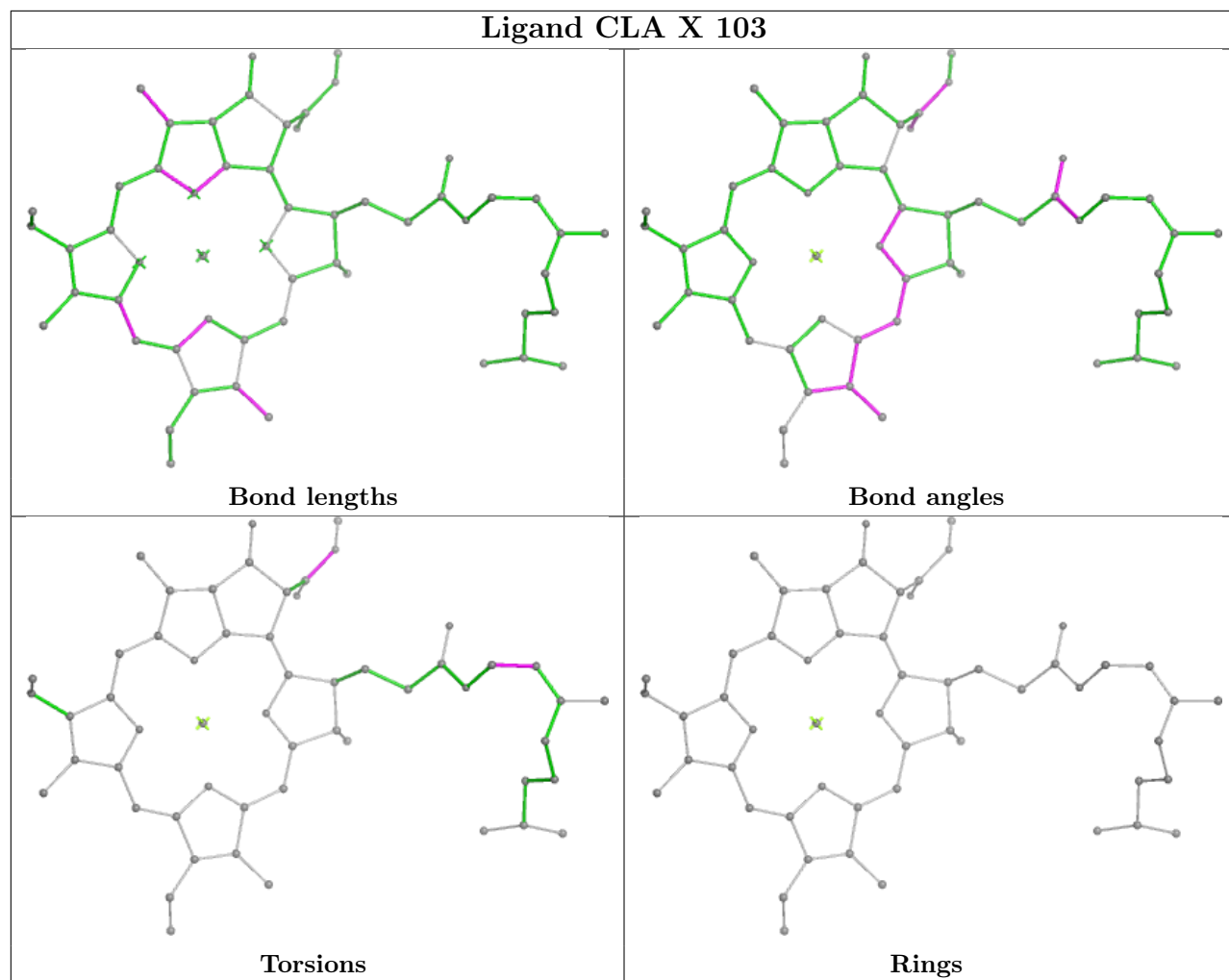






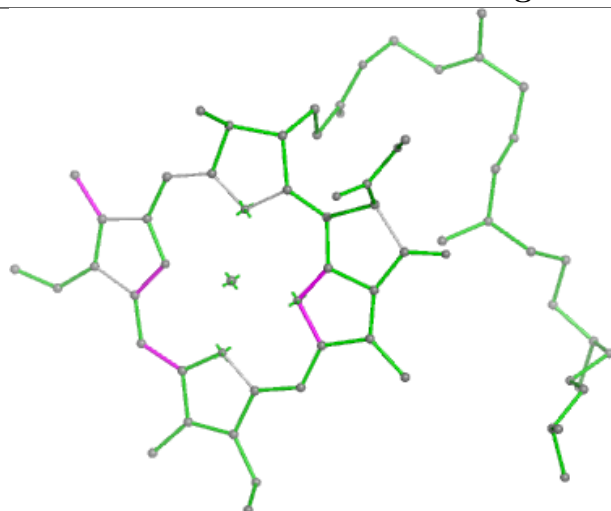




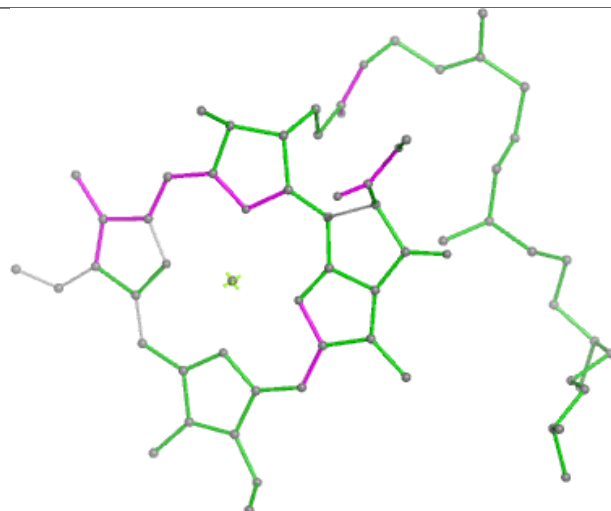




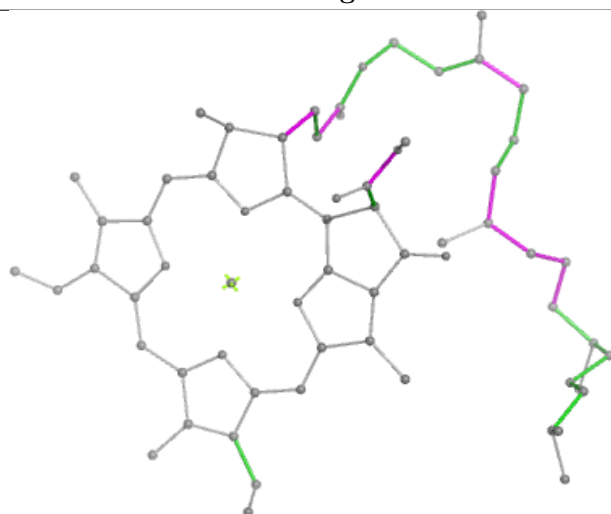
## Ligand CLA B 830



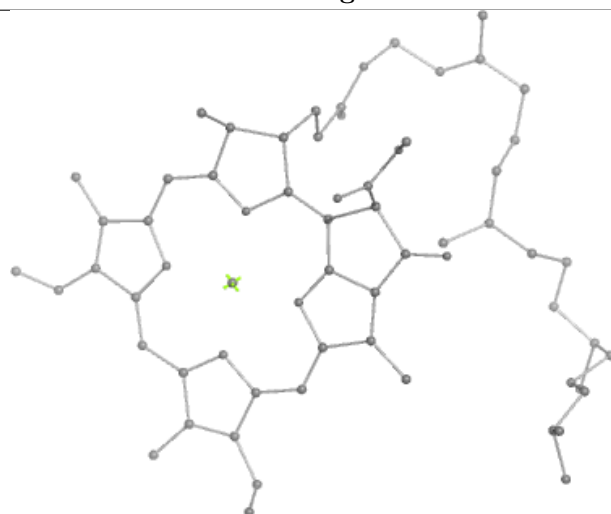
Bond lengths



Bond angles

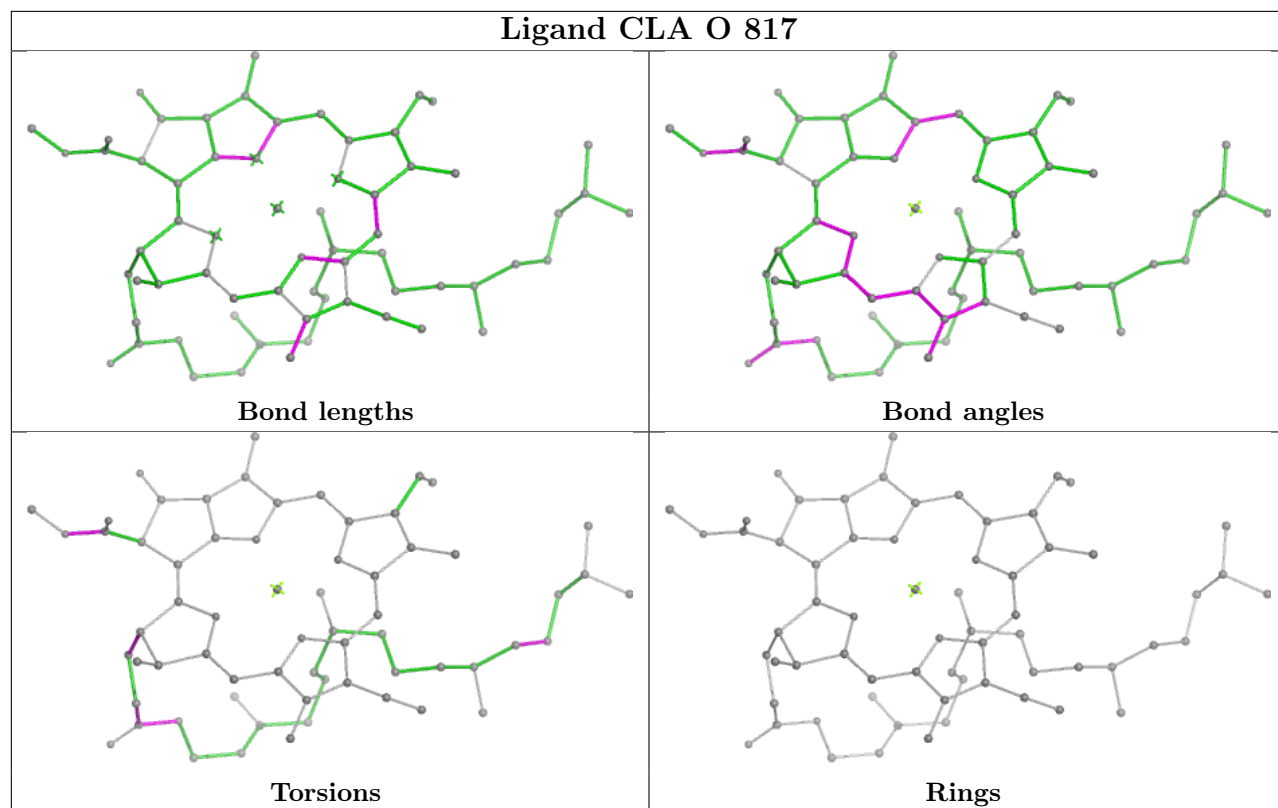


Torsions



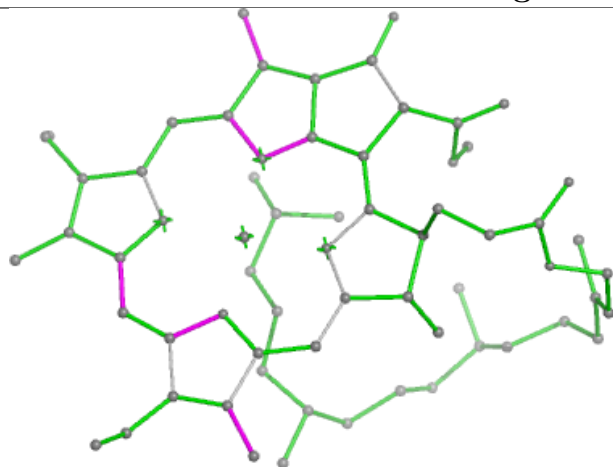
Rings



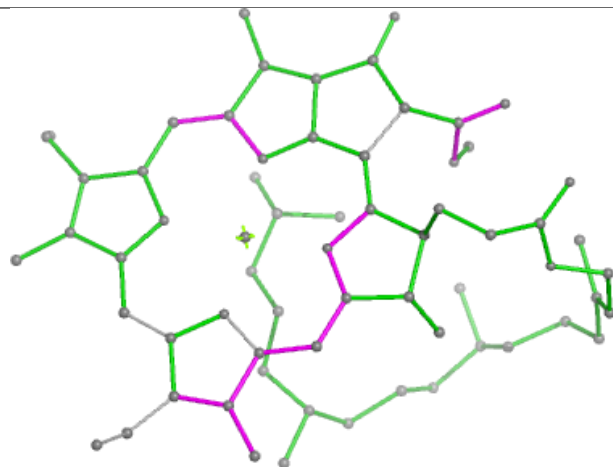




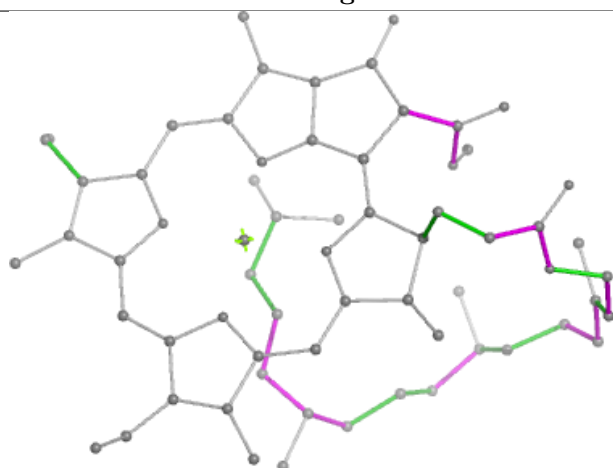
## Ligand CLA N 807



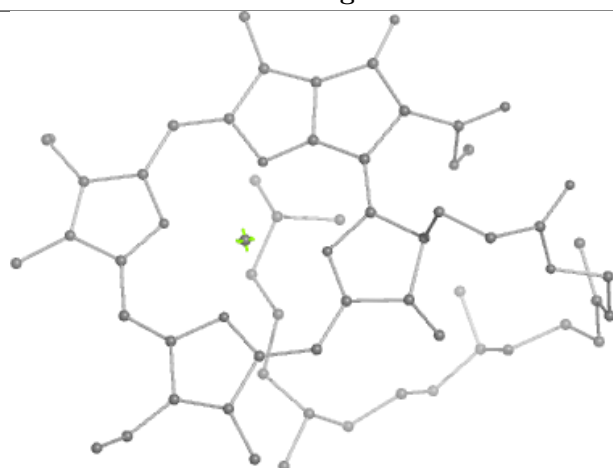
Bond lengths



Bond angles

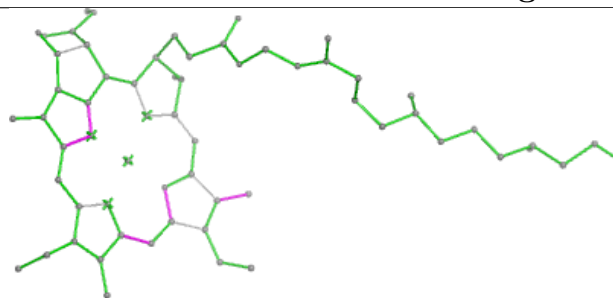


Torsions

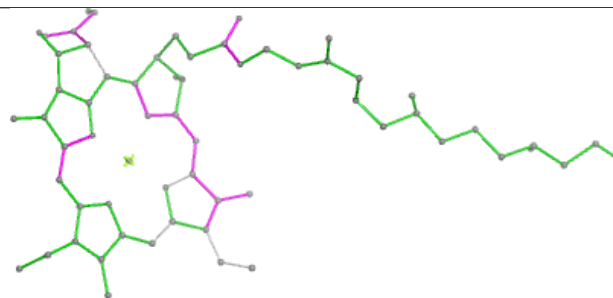


Rings

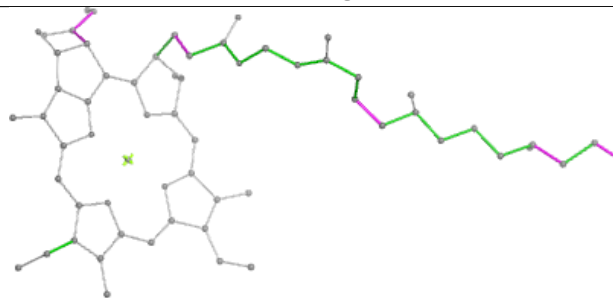
## Ligand CLA a 835



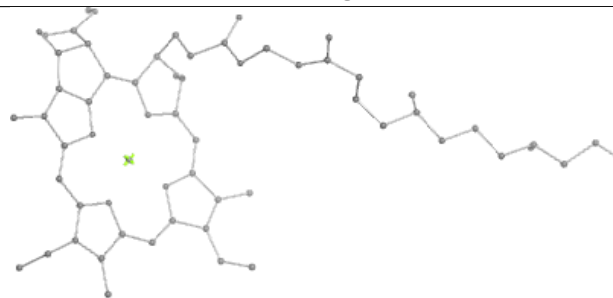
Bond lengths



Bond angles

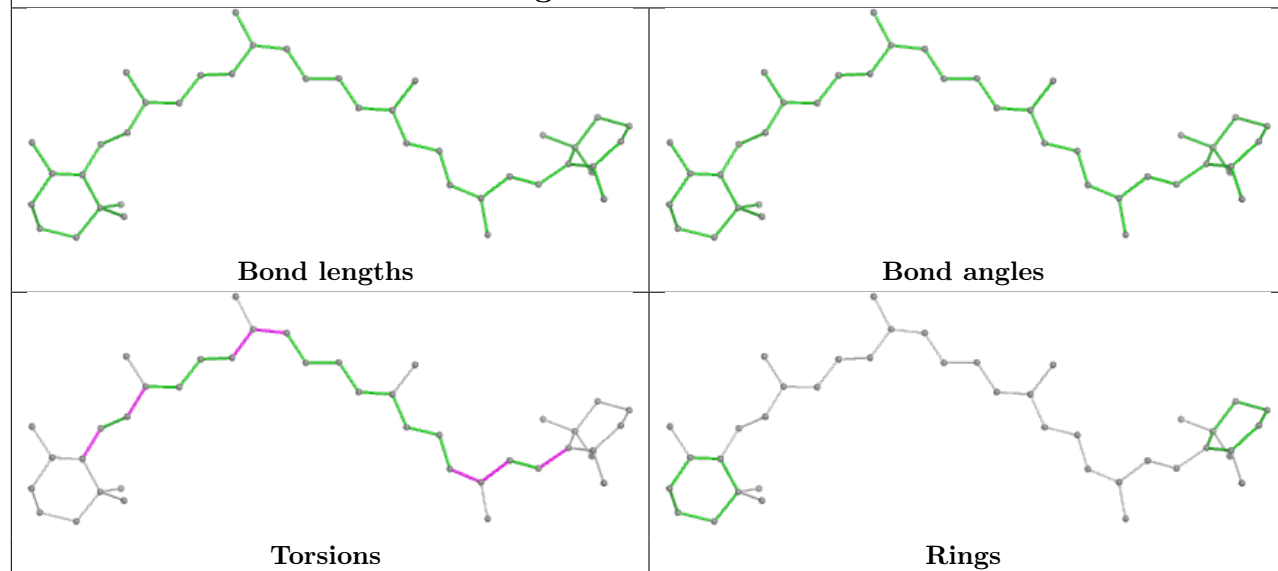
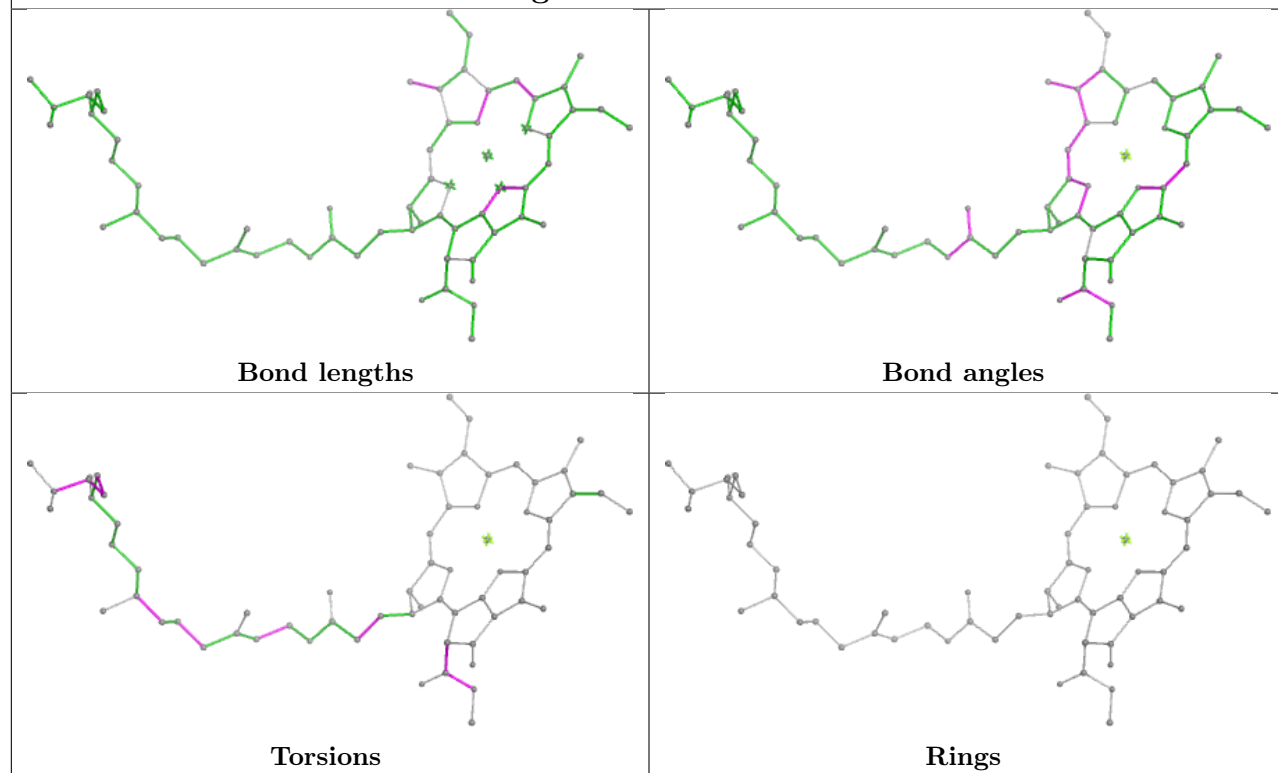


Torsions



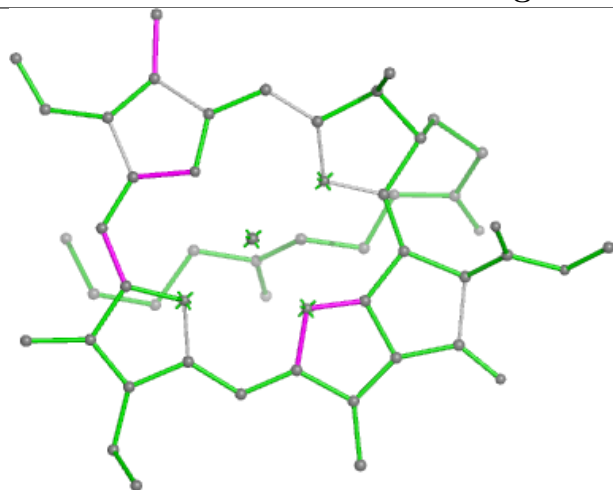
Rings



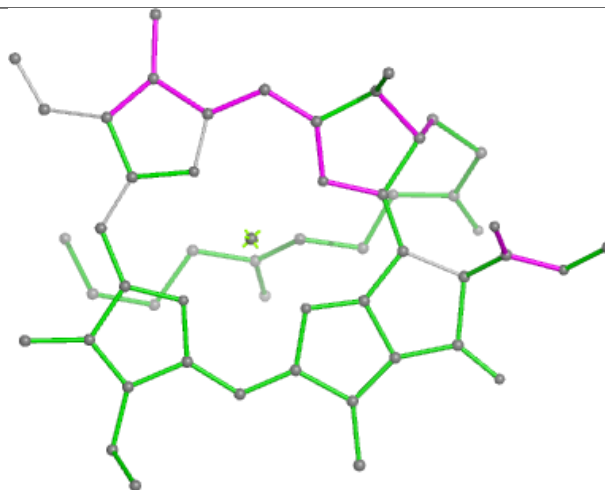
**Ligand BCR a 850****Ligand CLA O 802**



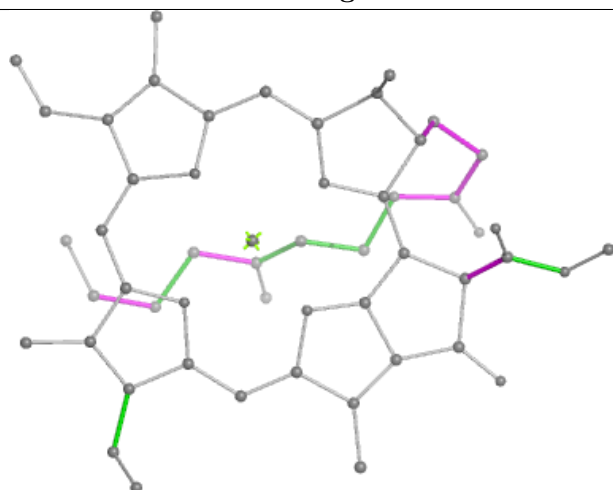
## Ligand CLA O 822



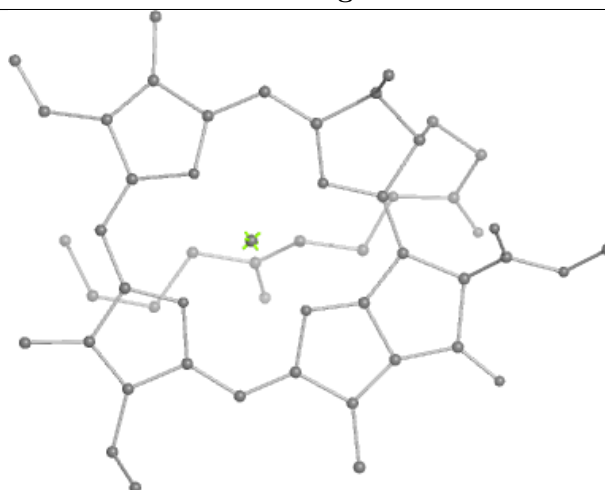
Bond lengths



Bond angles

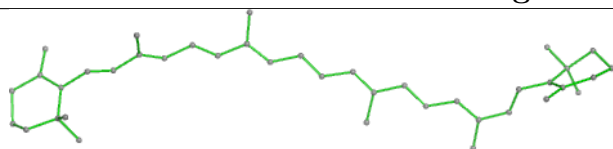


Torsions

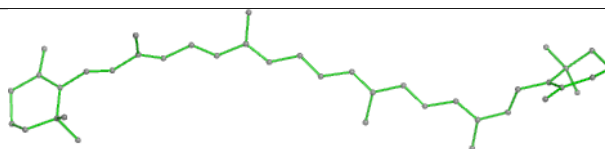


Rings

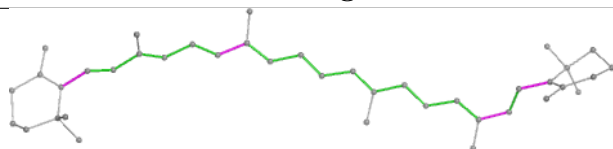
## Ligand BCR B 844



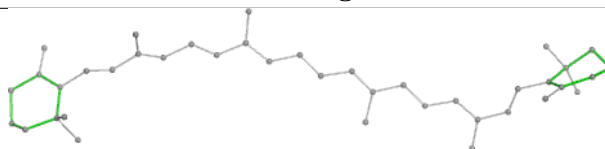
Bond lengths



Bond angles

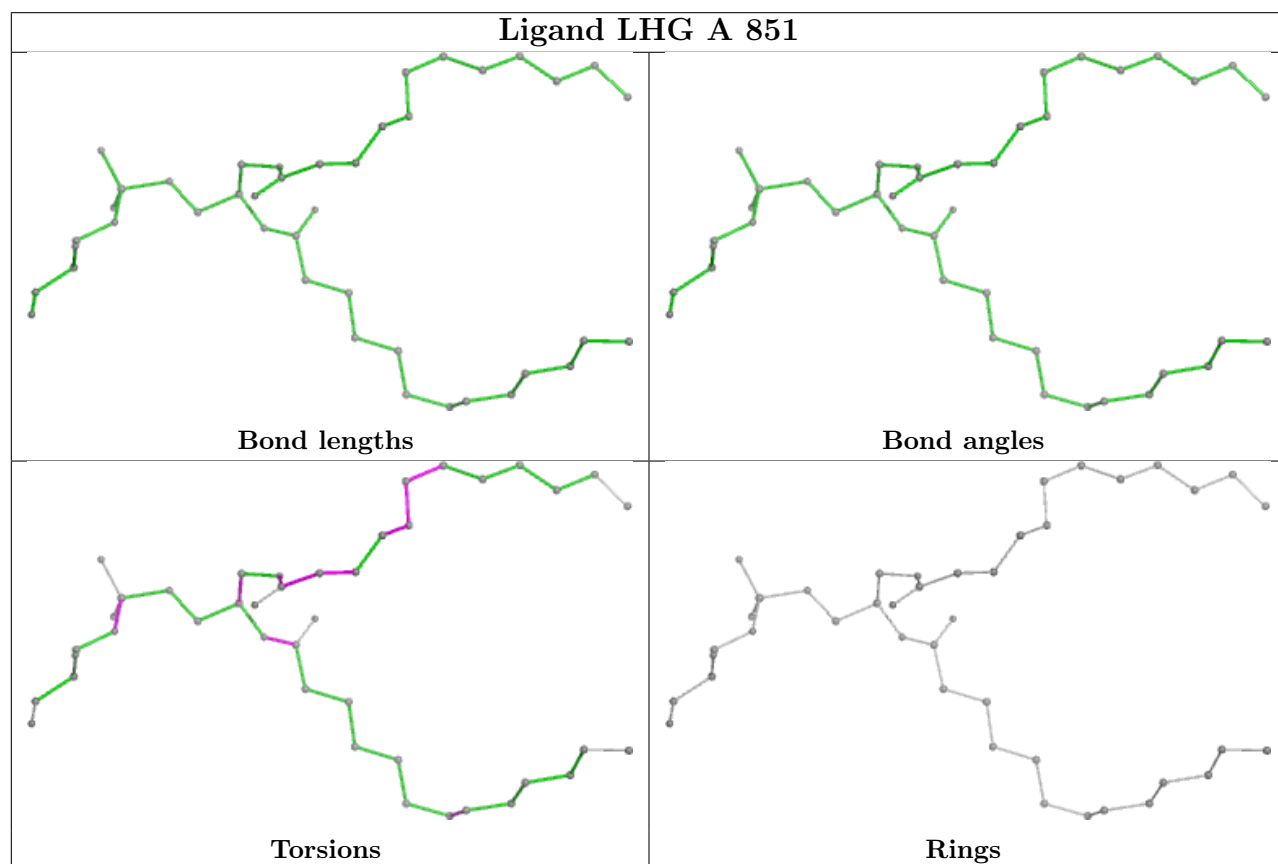
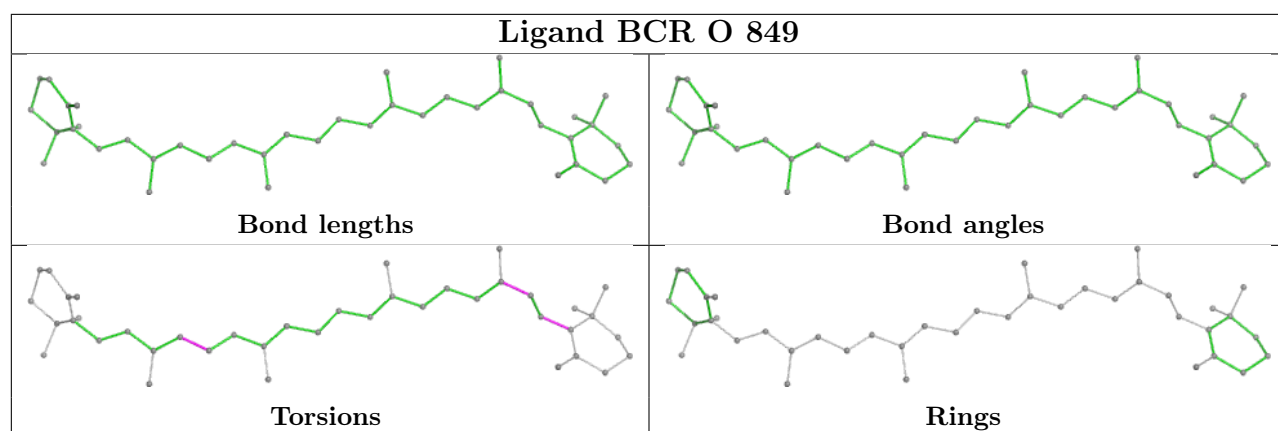


Torsions

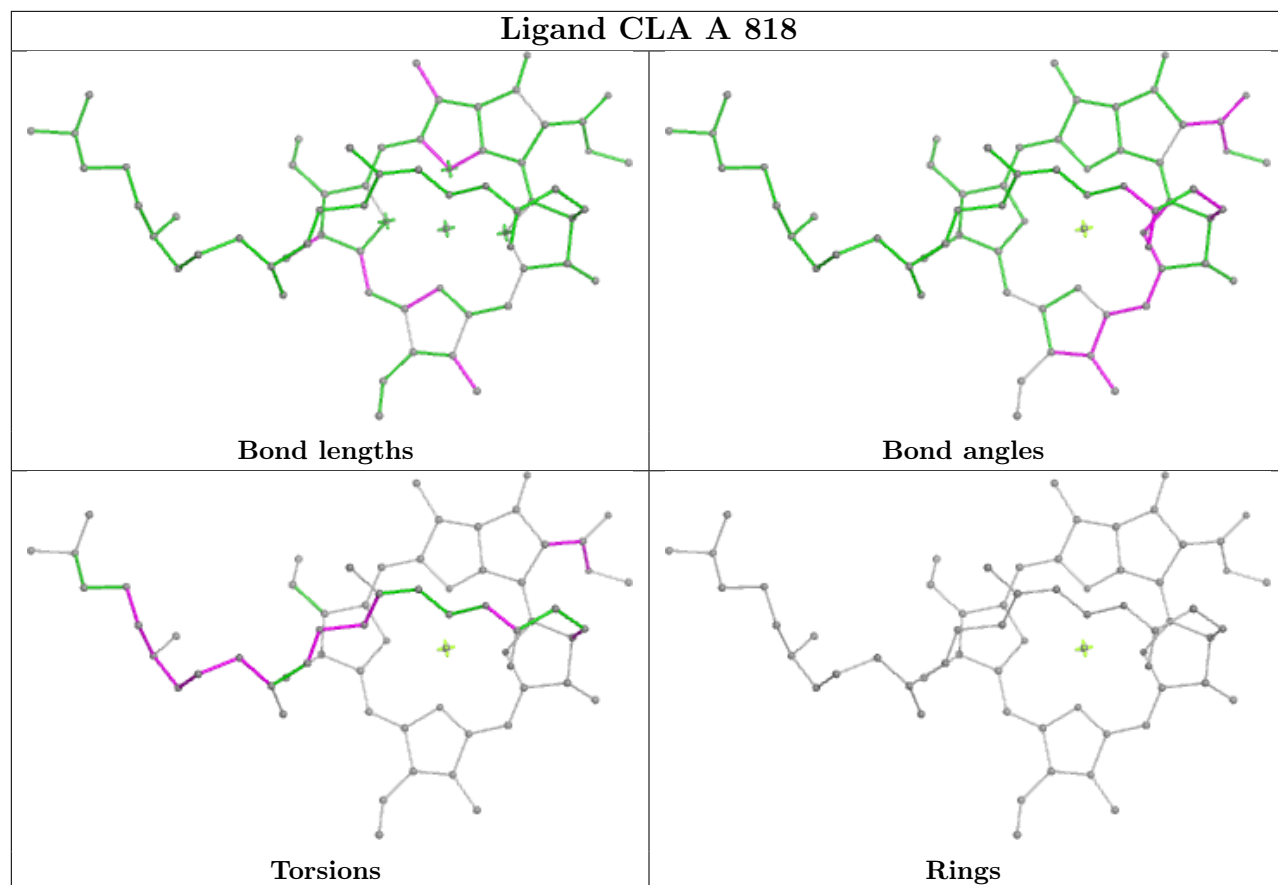
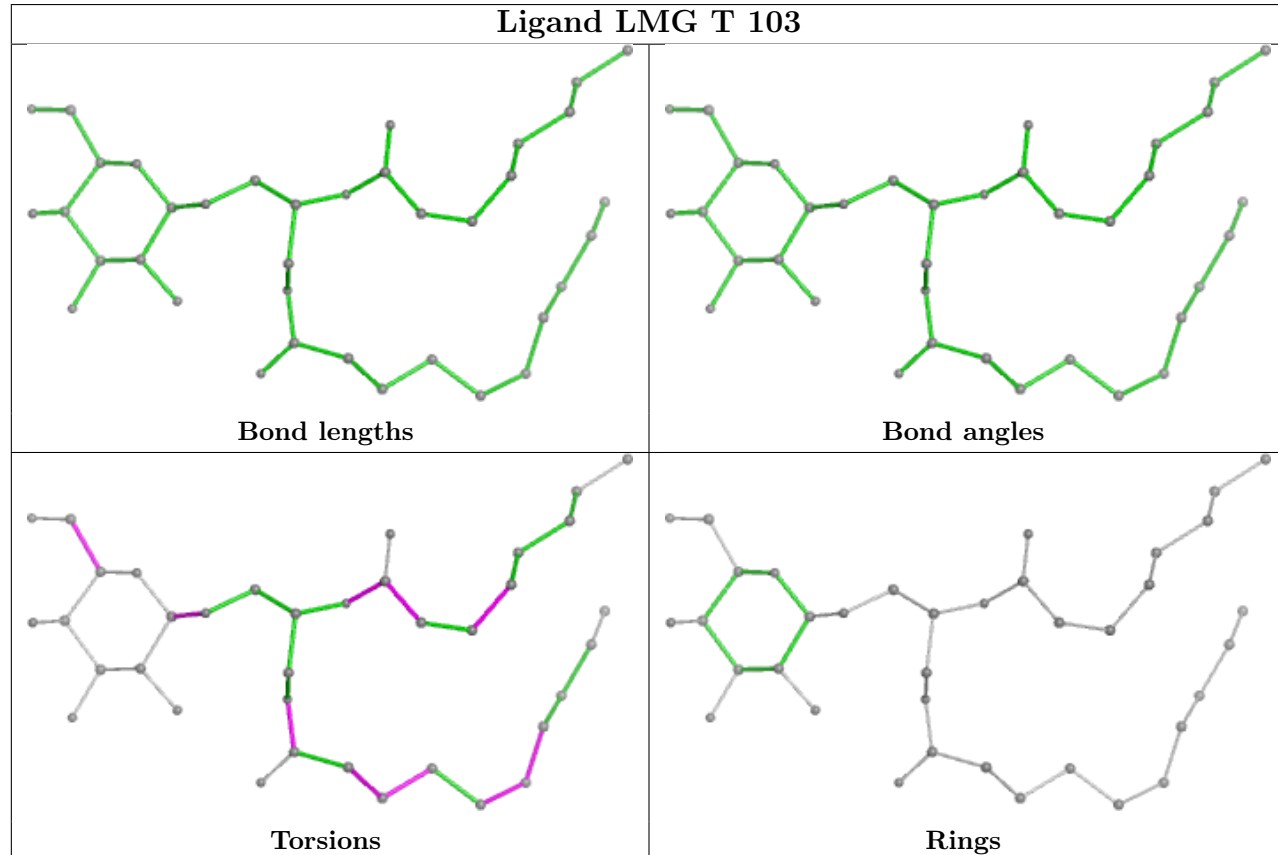


Rings

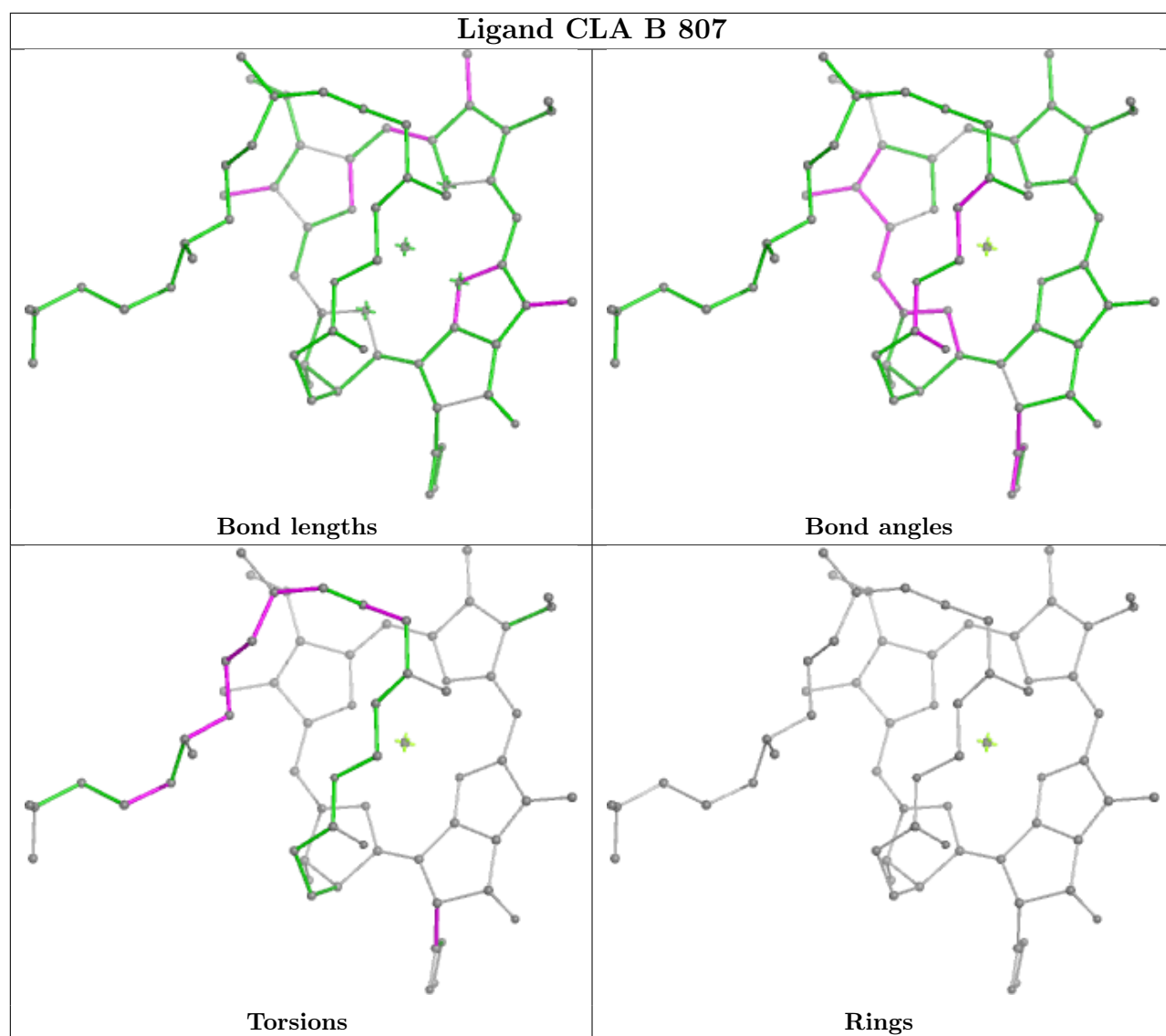






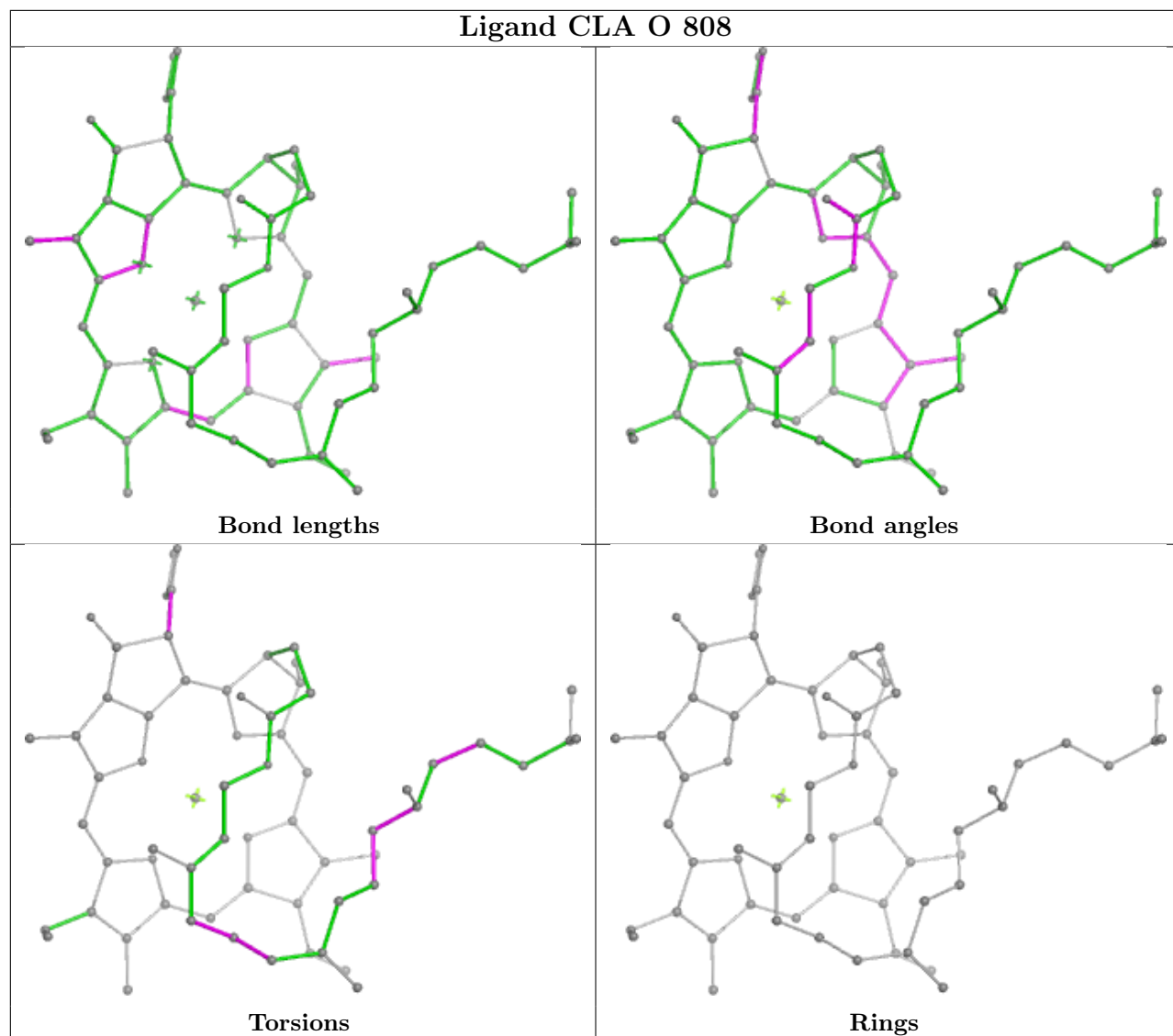
**Ligand CLA A 818****Ligand LMG T 103**



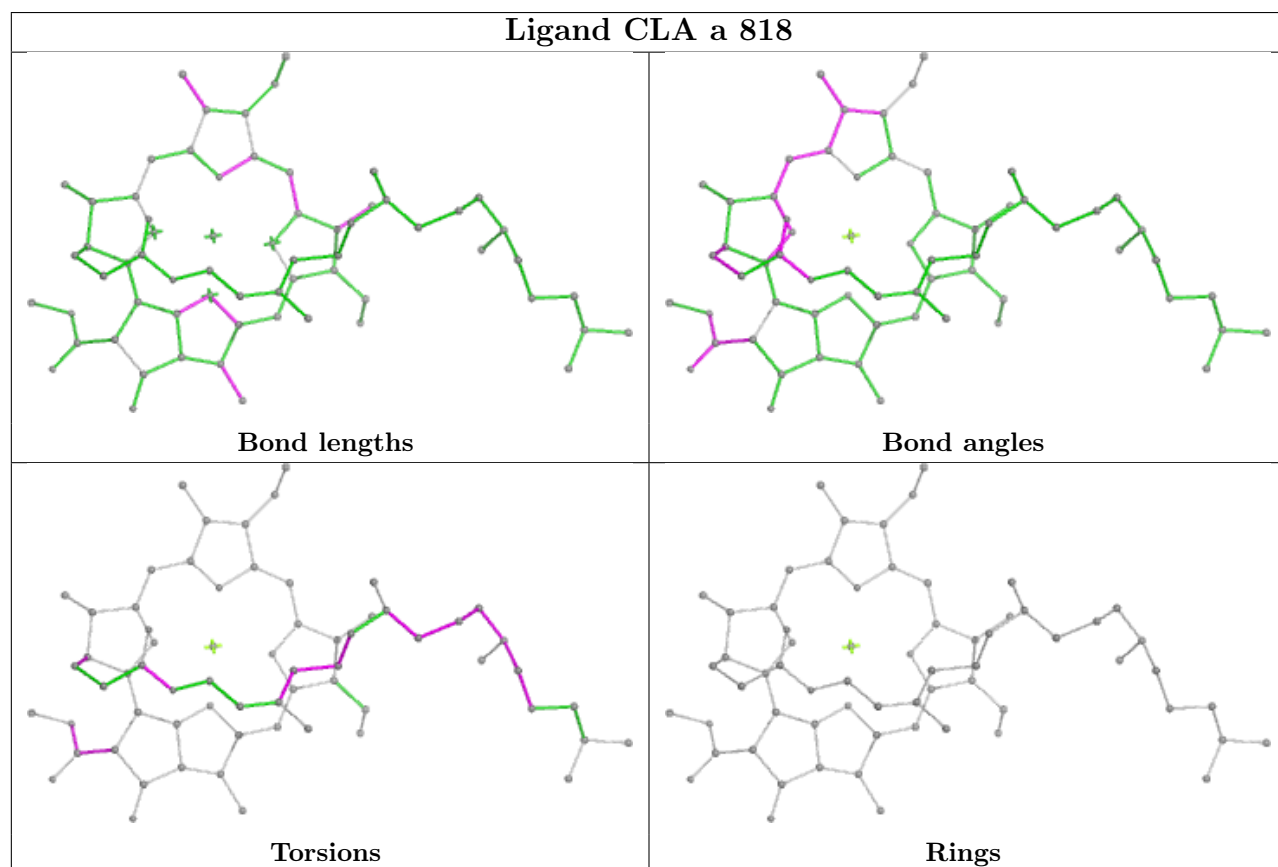
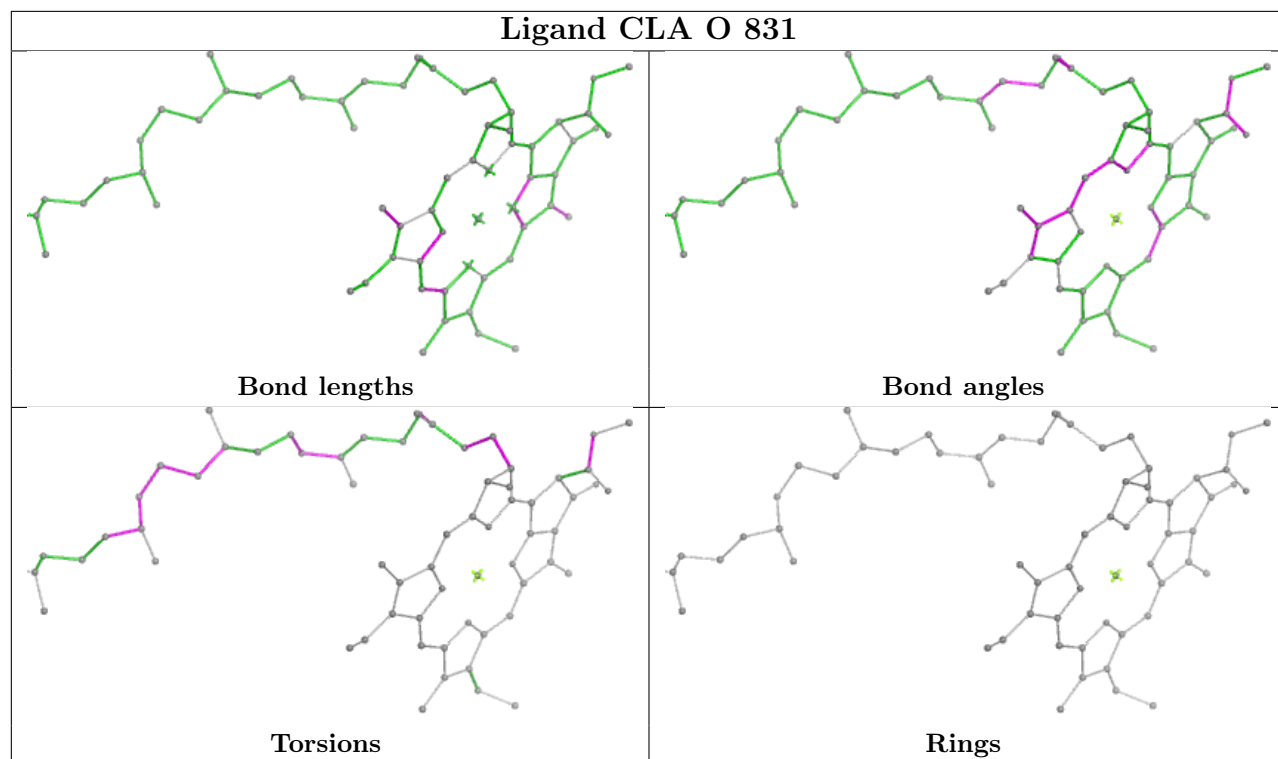




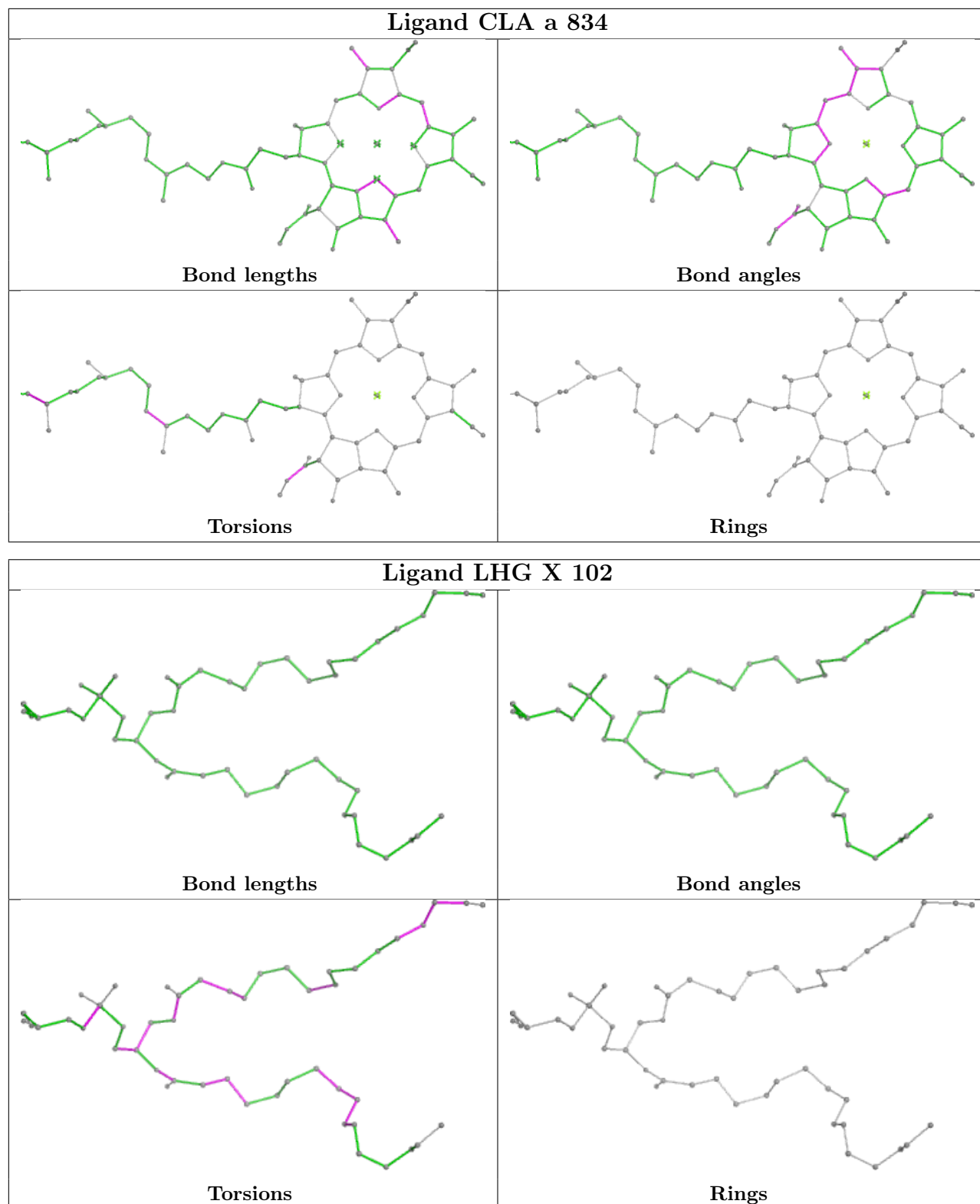
## Ligand CLA O 808



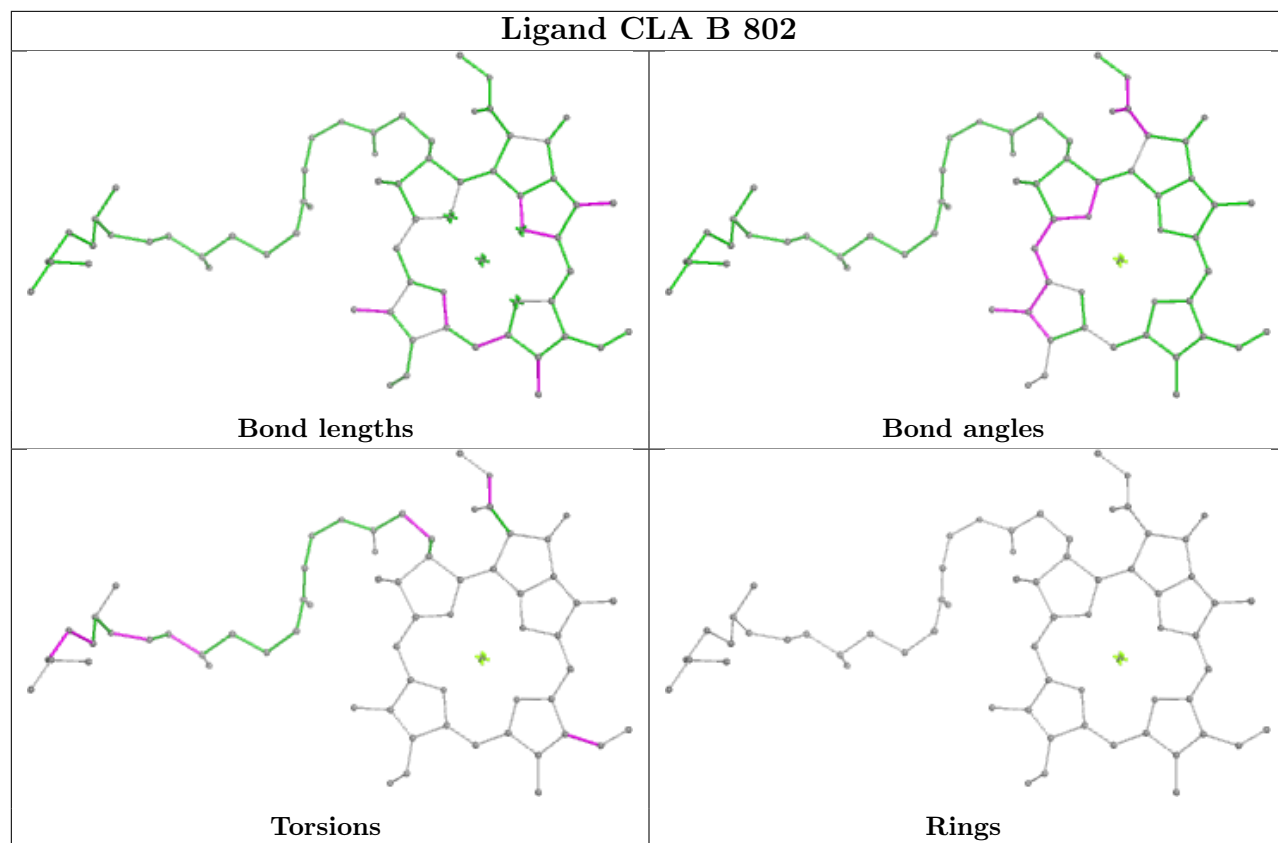






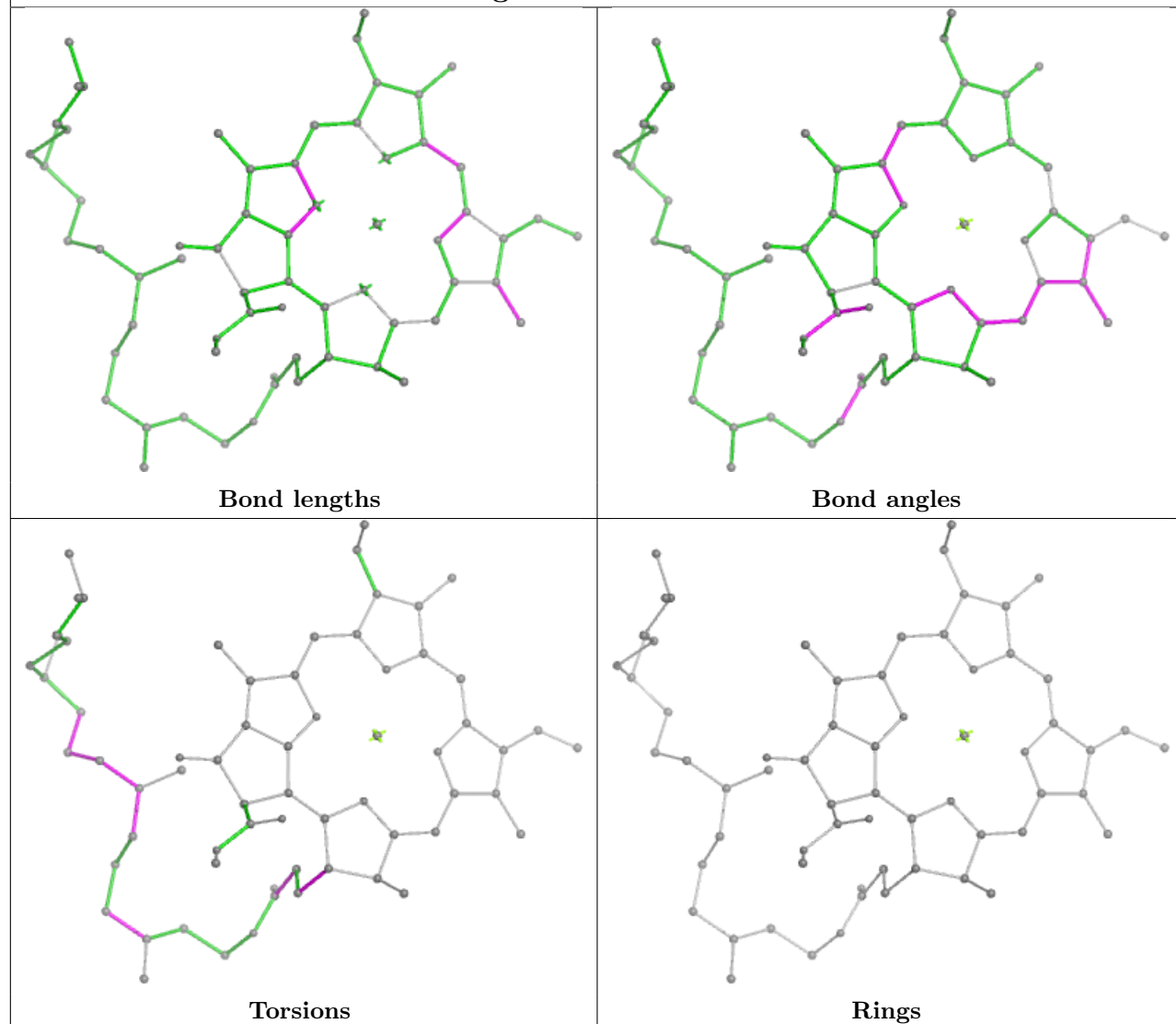




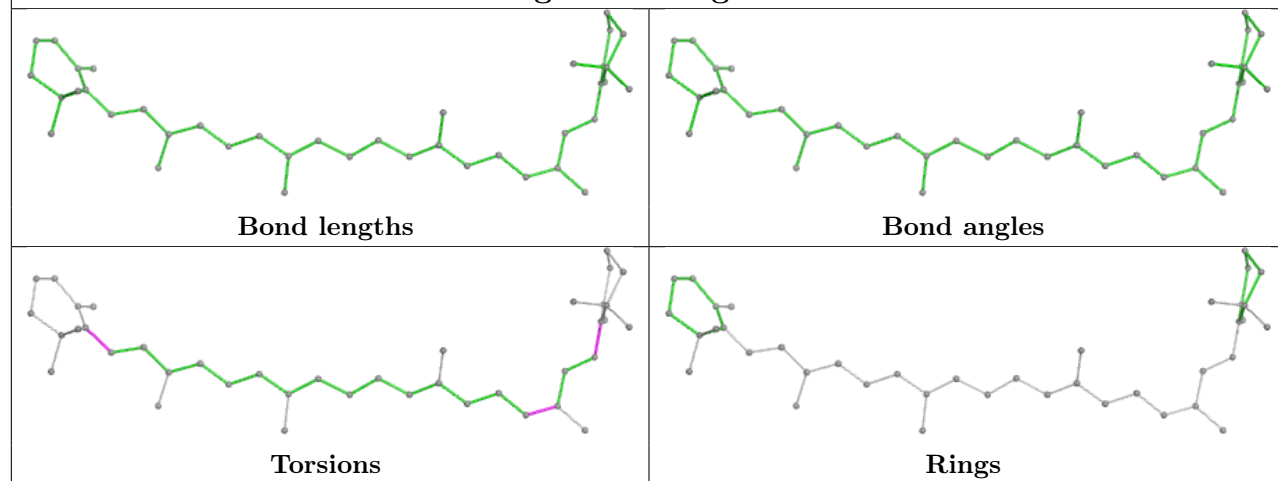




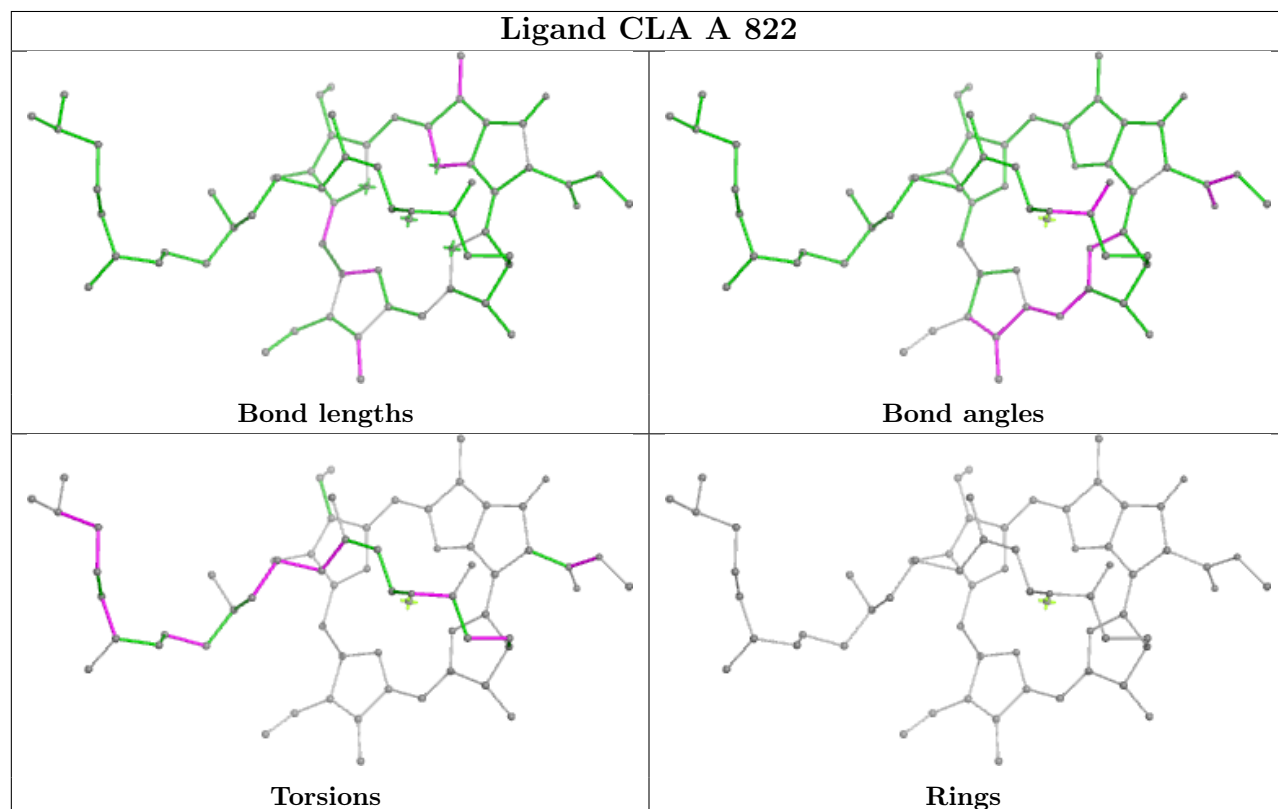
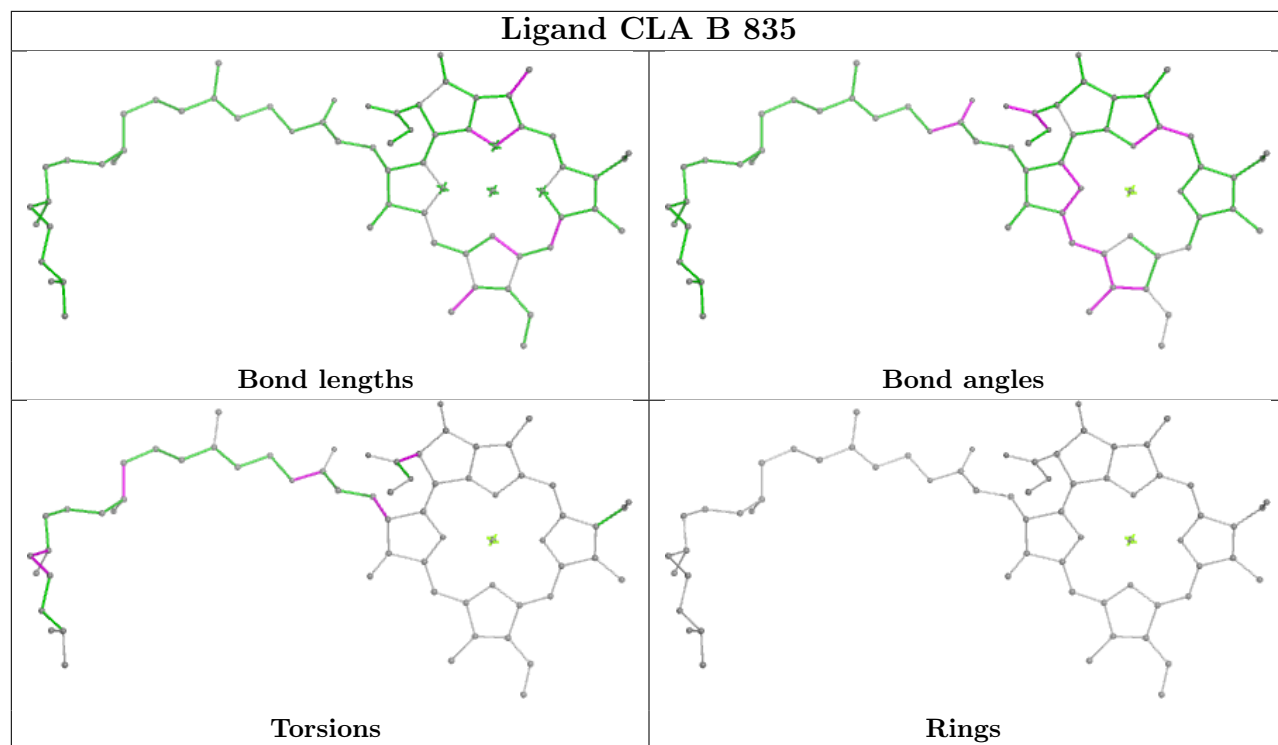
## Ligand CLA b 832



## Ligand BCR g 102

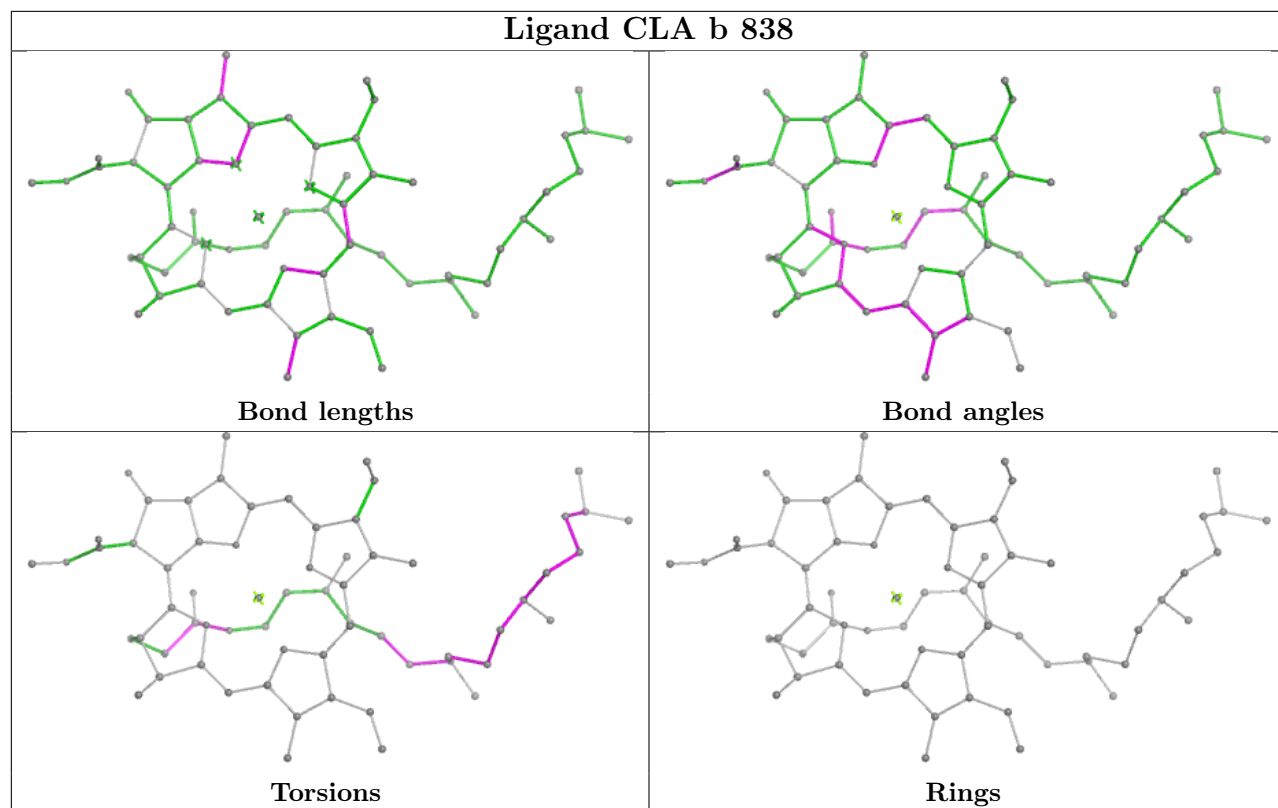




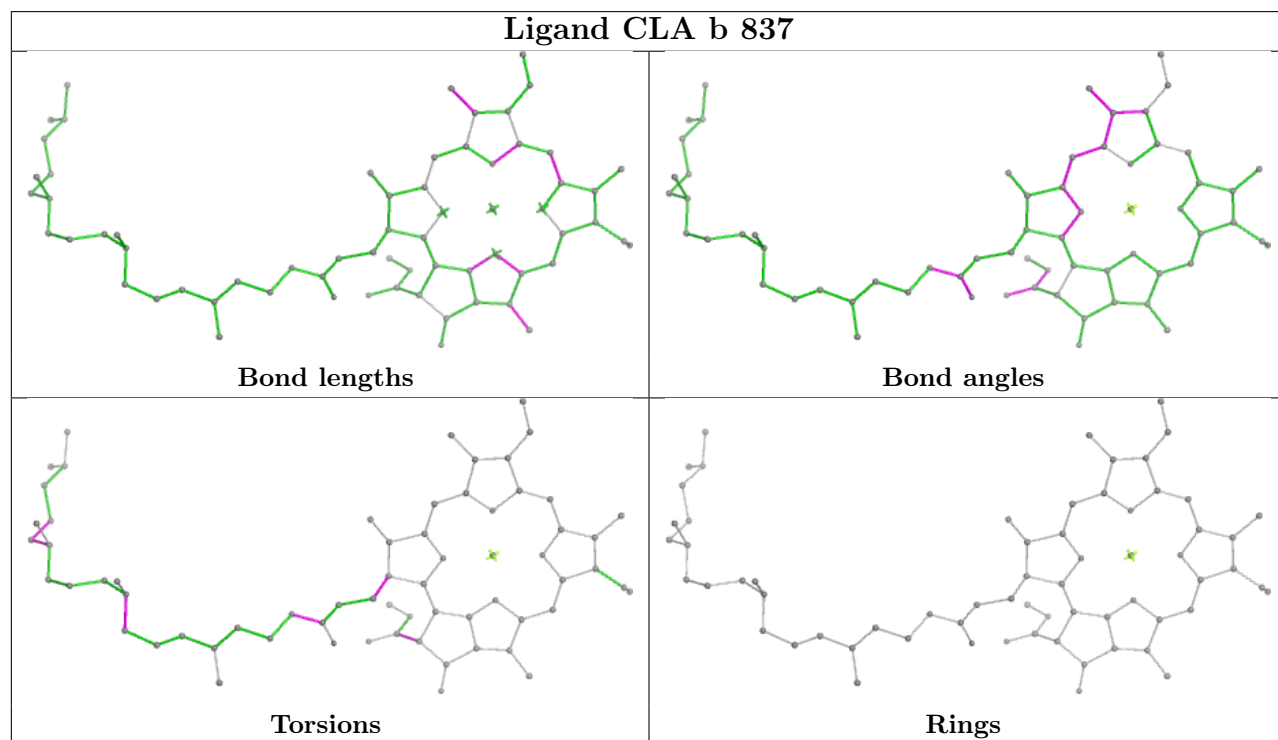




## Ligand CLA b 838

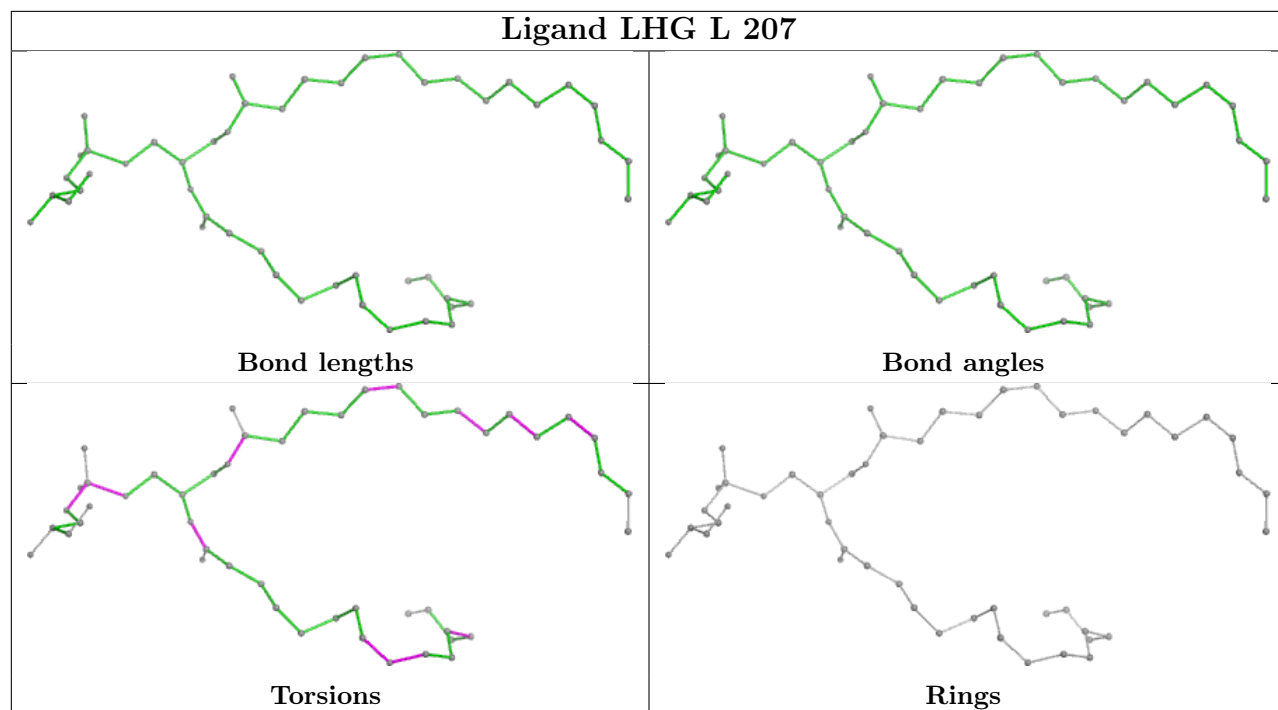


## Ligand CLA b 837

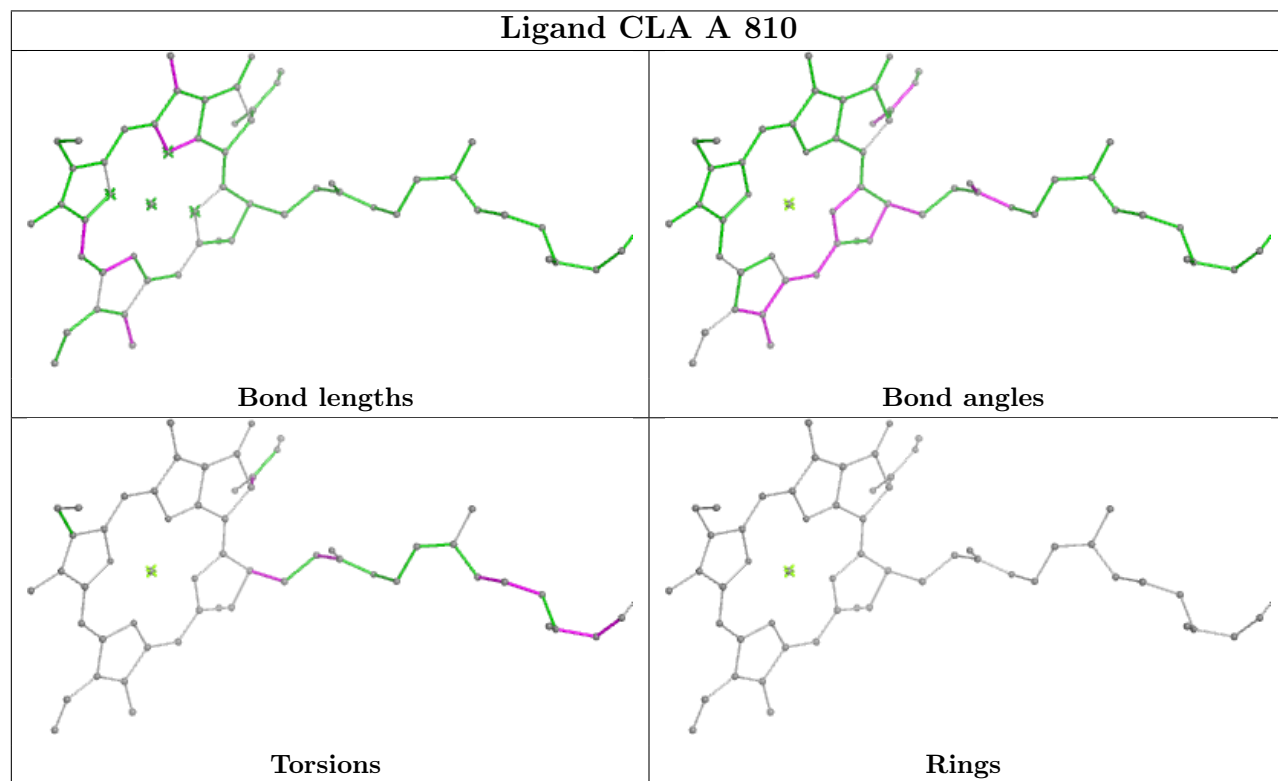




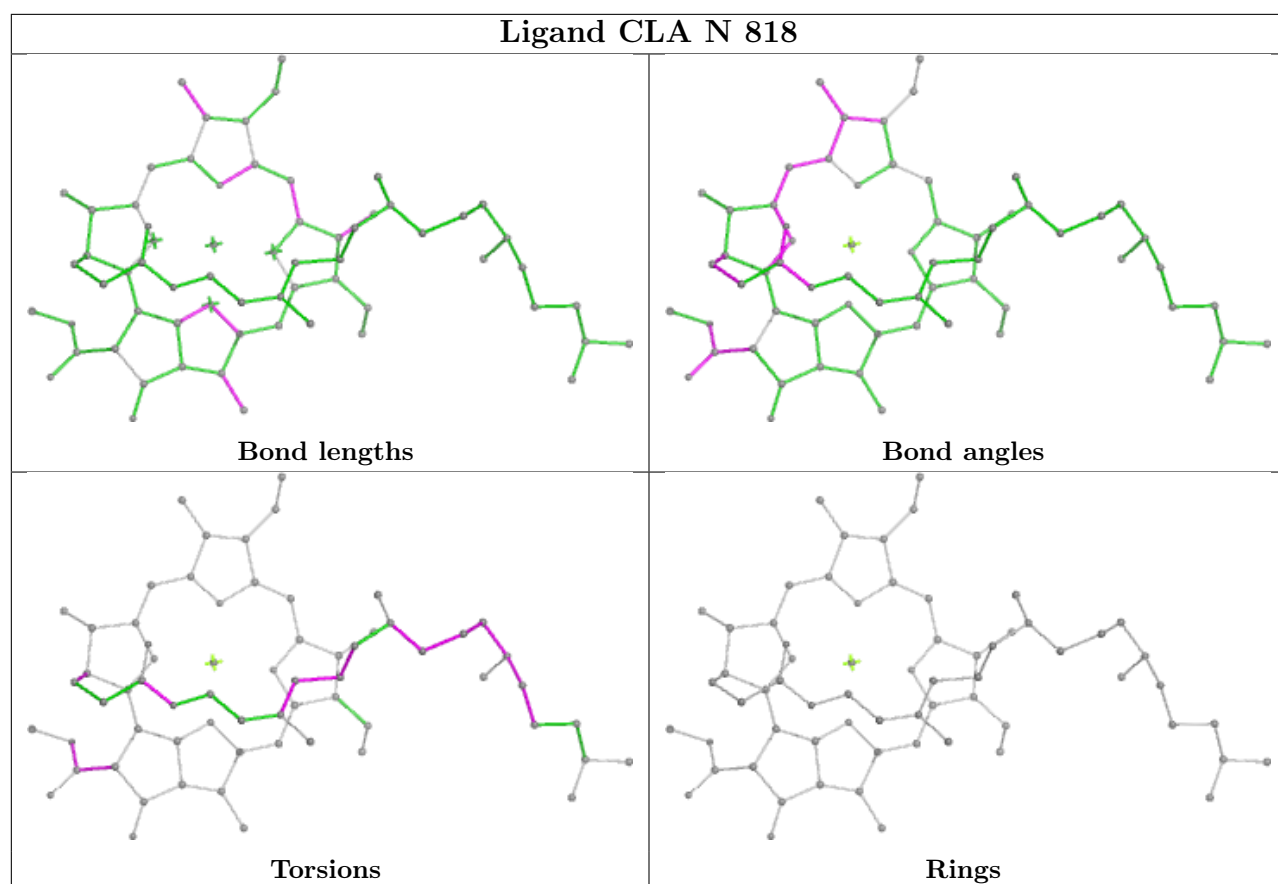
## Ligand LHG L 207



## Ligand CLA A 810

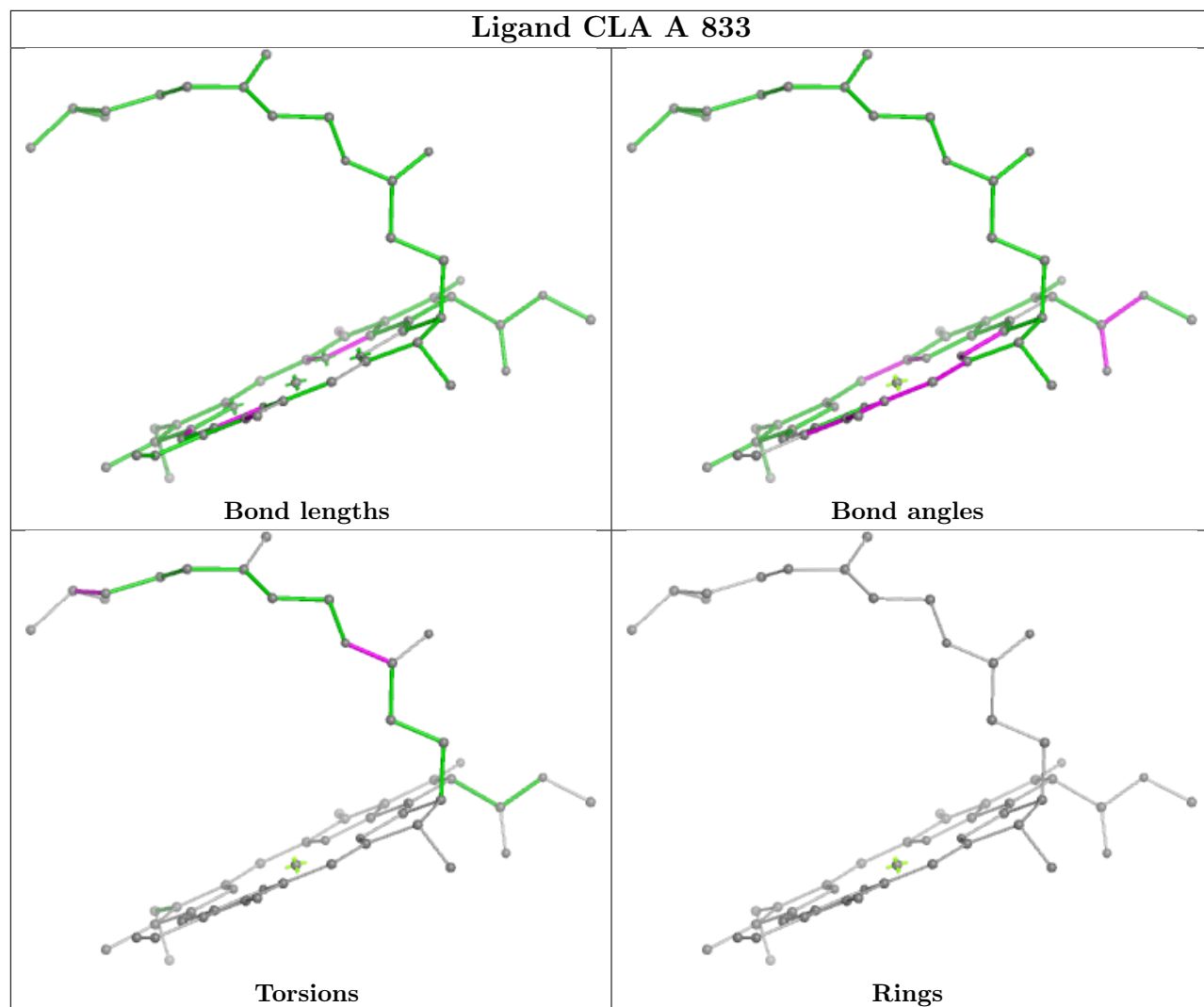






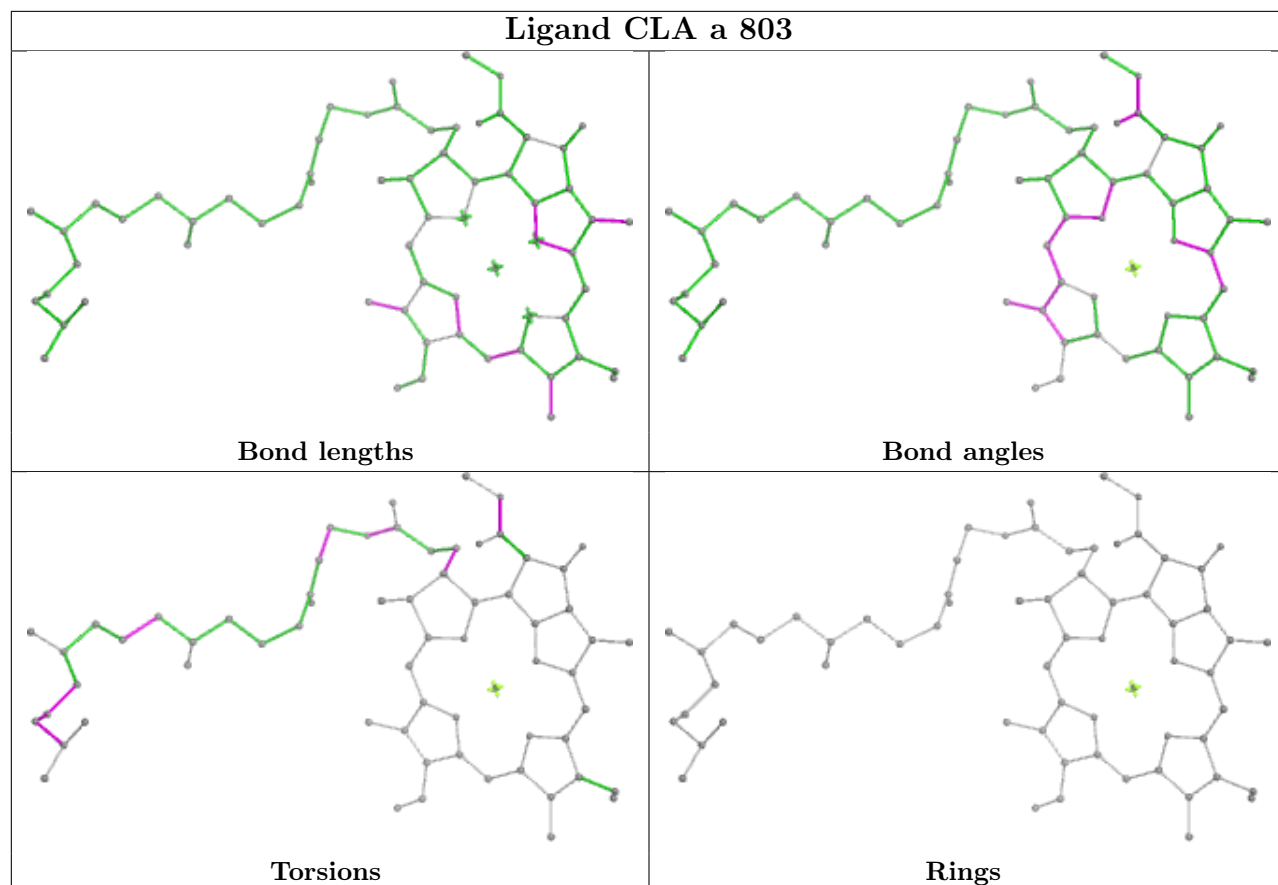


## Ligand CLA A 833

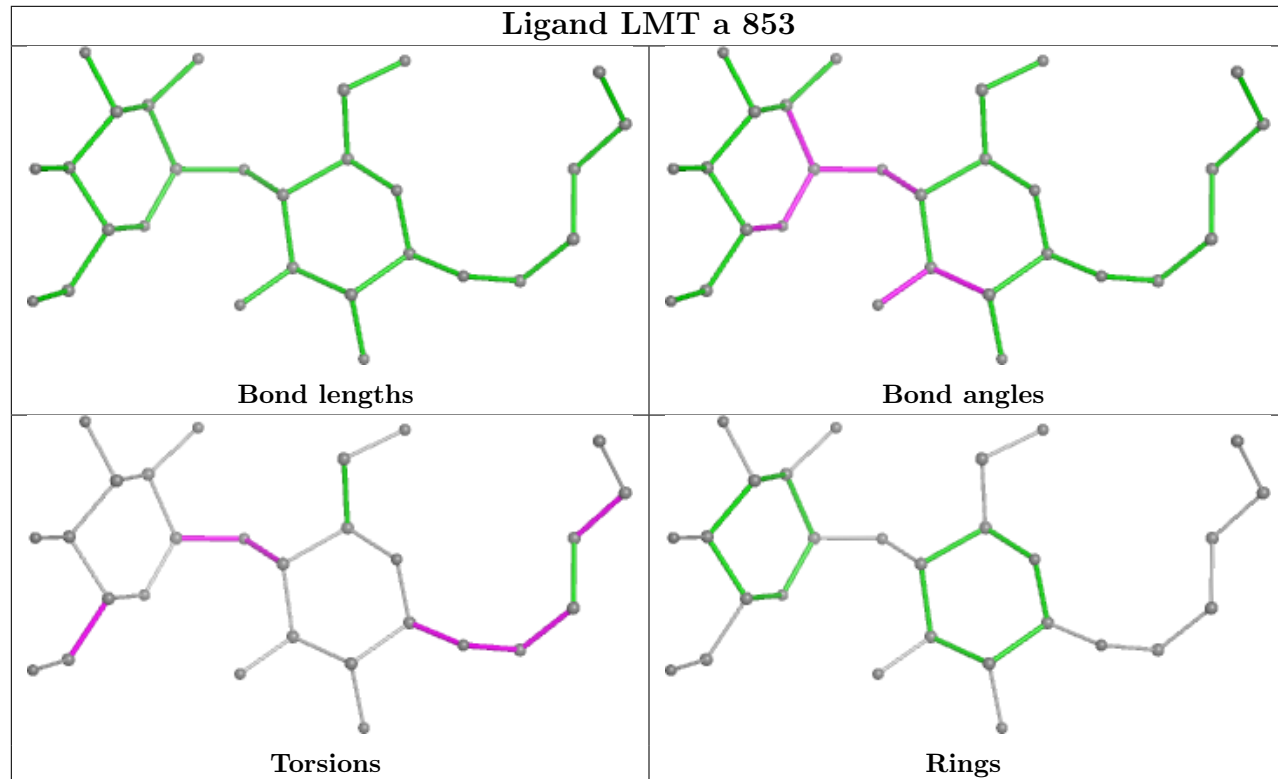




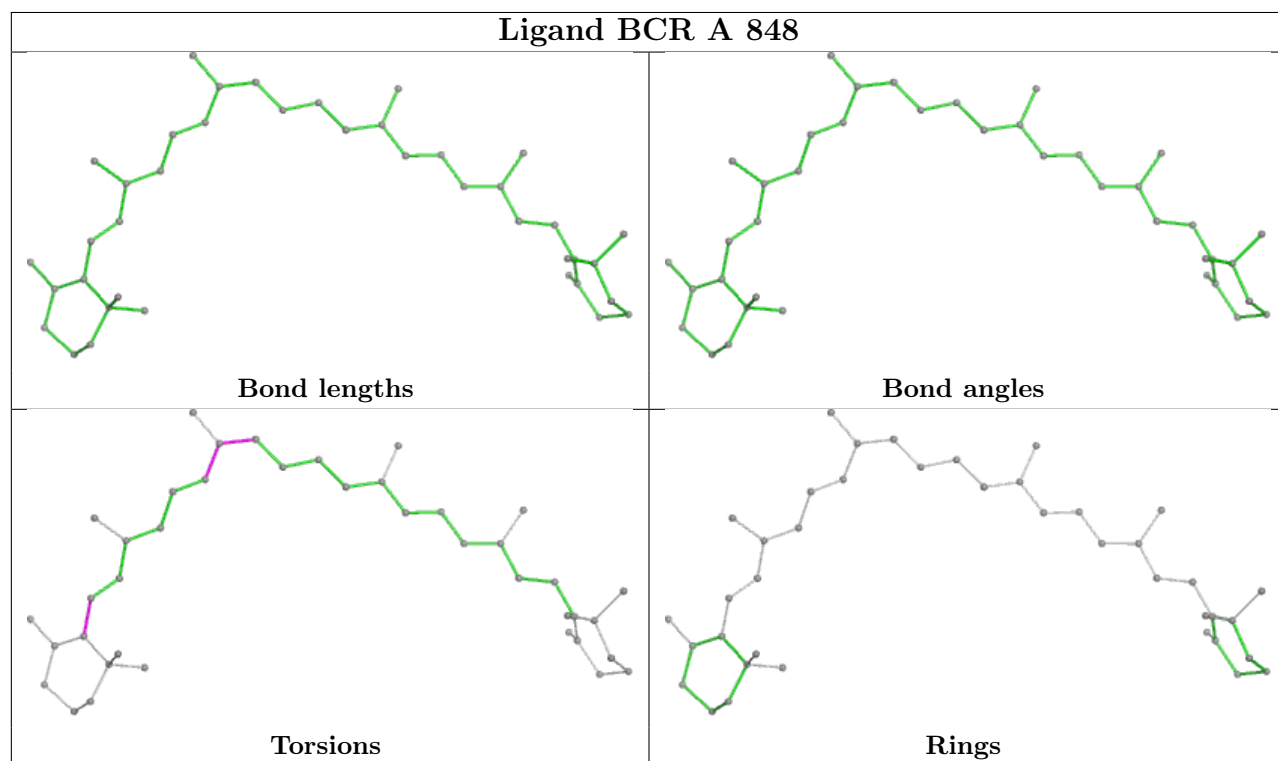
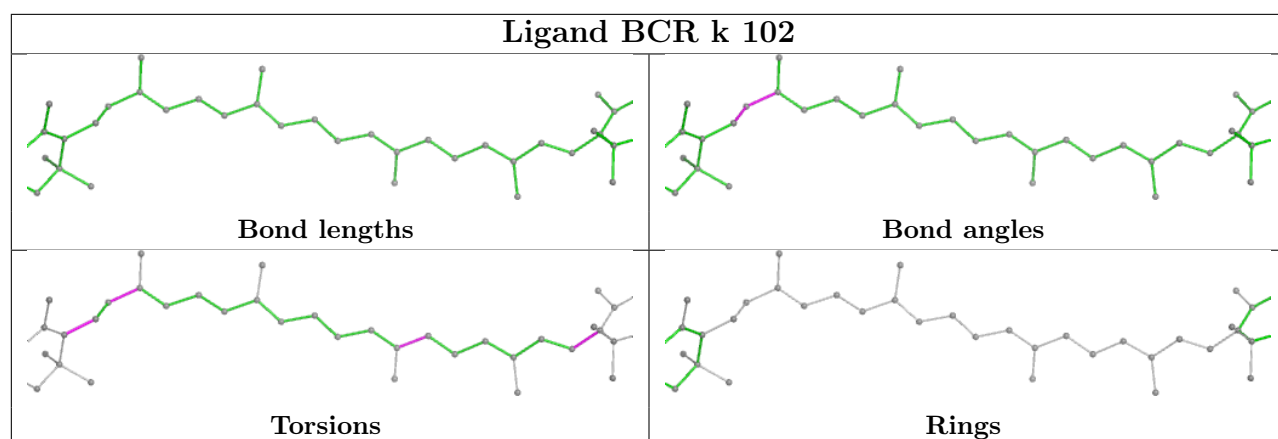
## Ligand CLA a 803



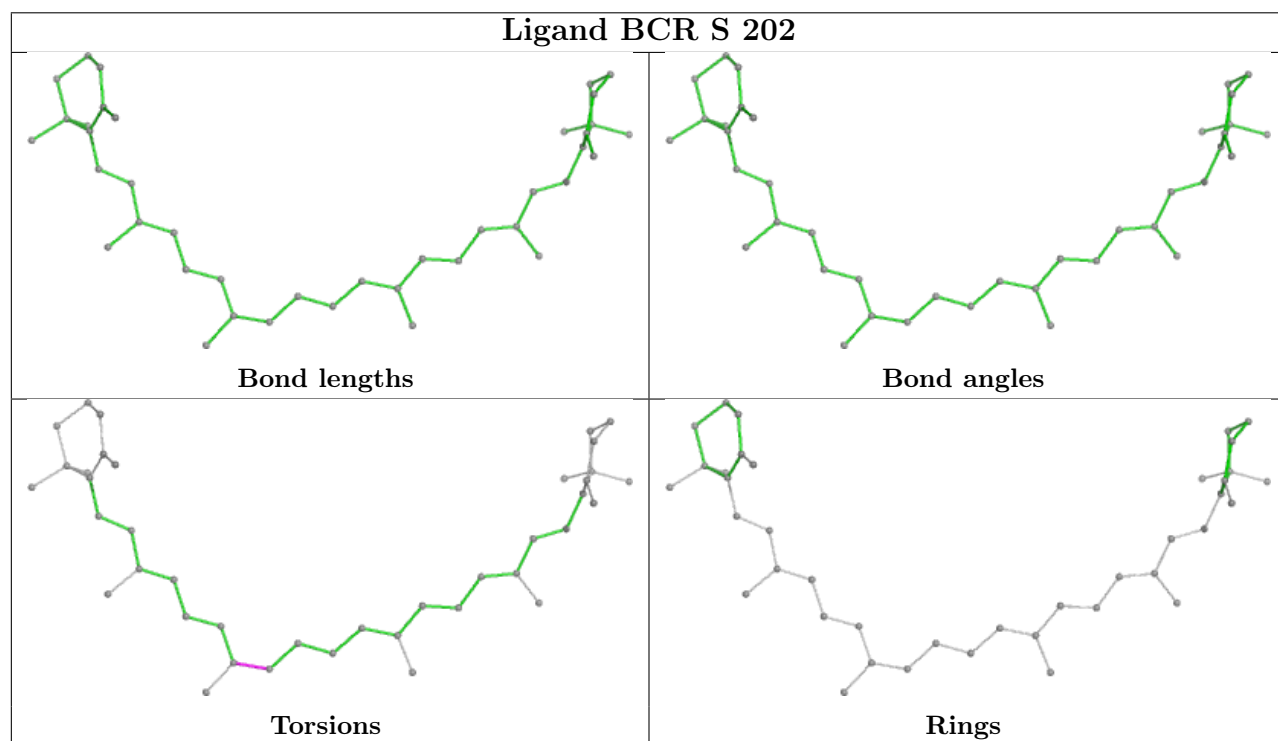
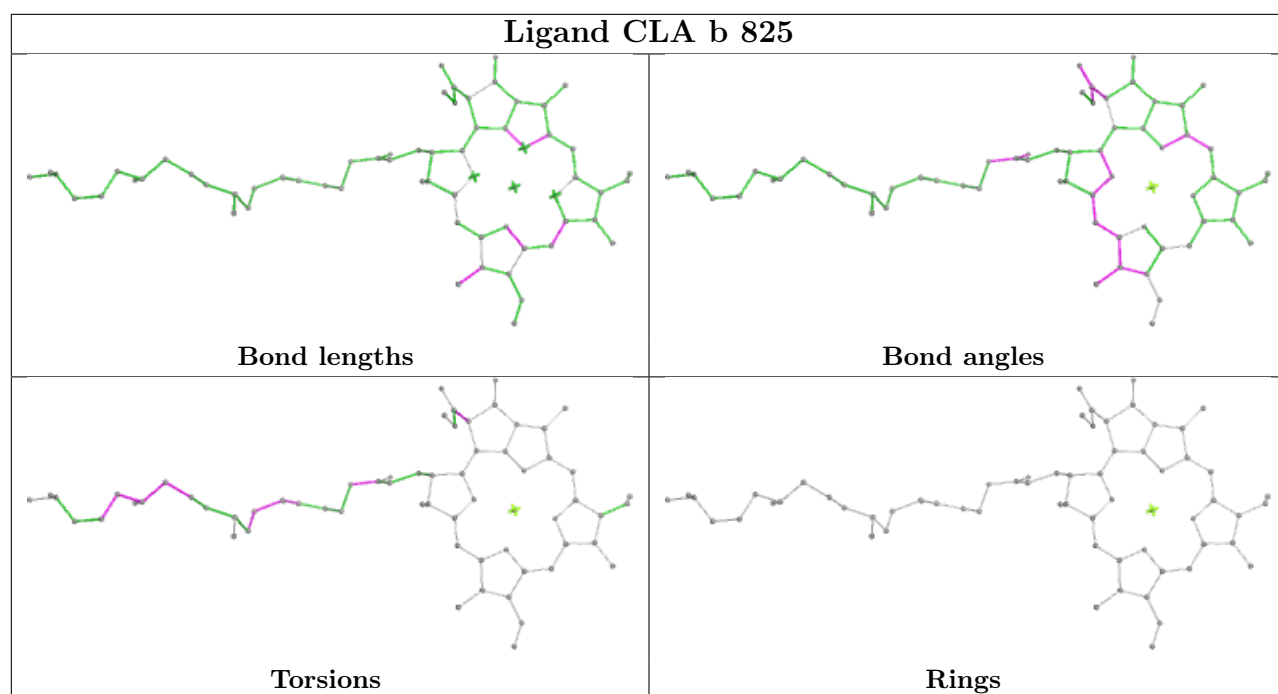
## Ligand LMT a 853





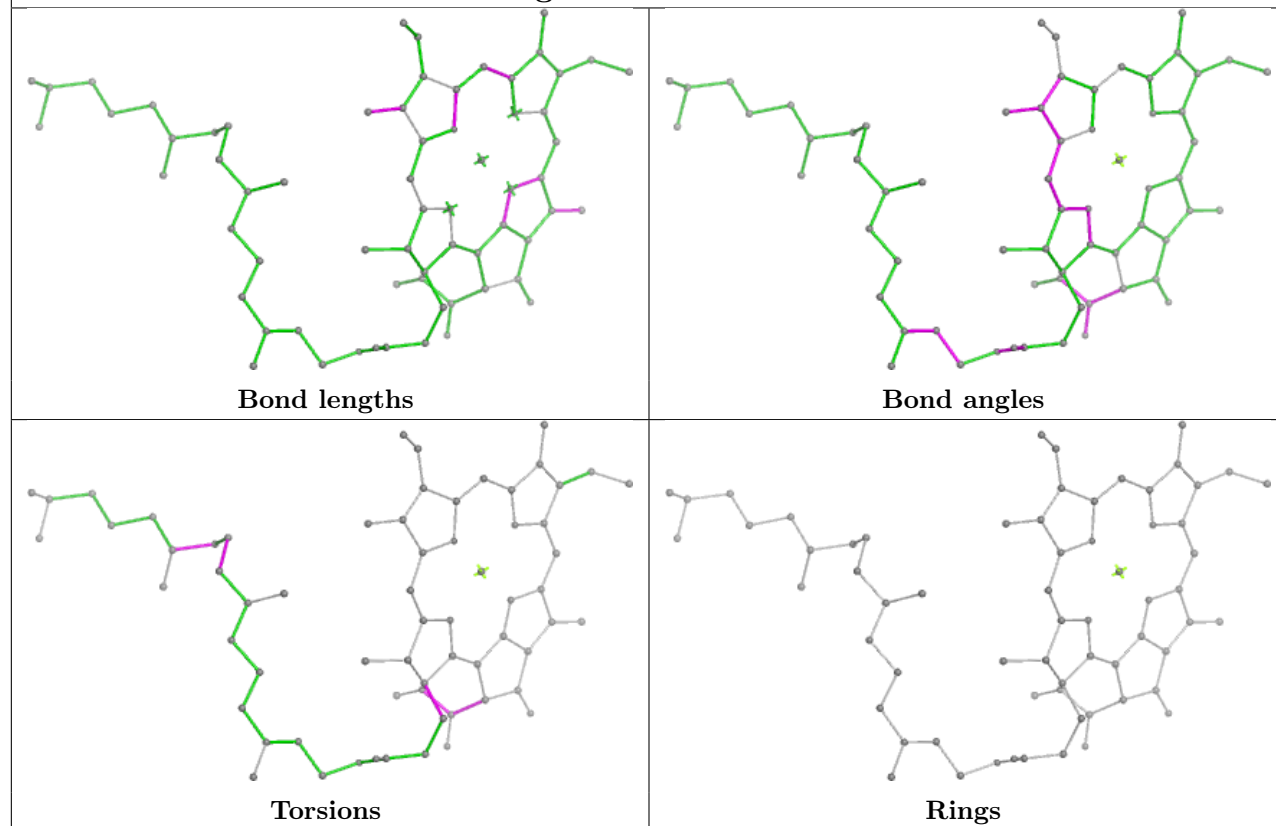




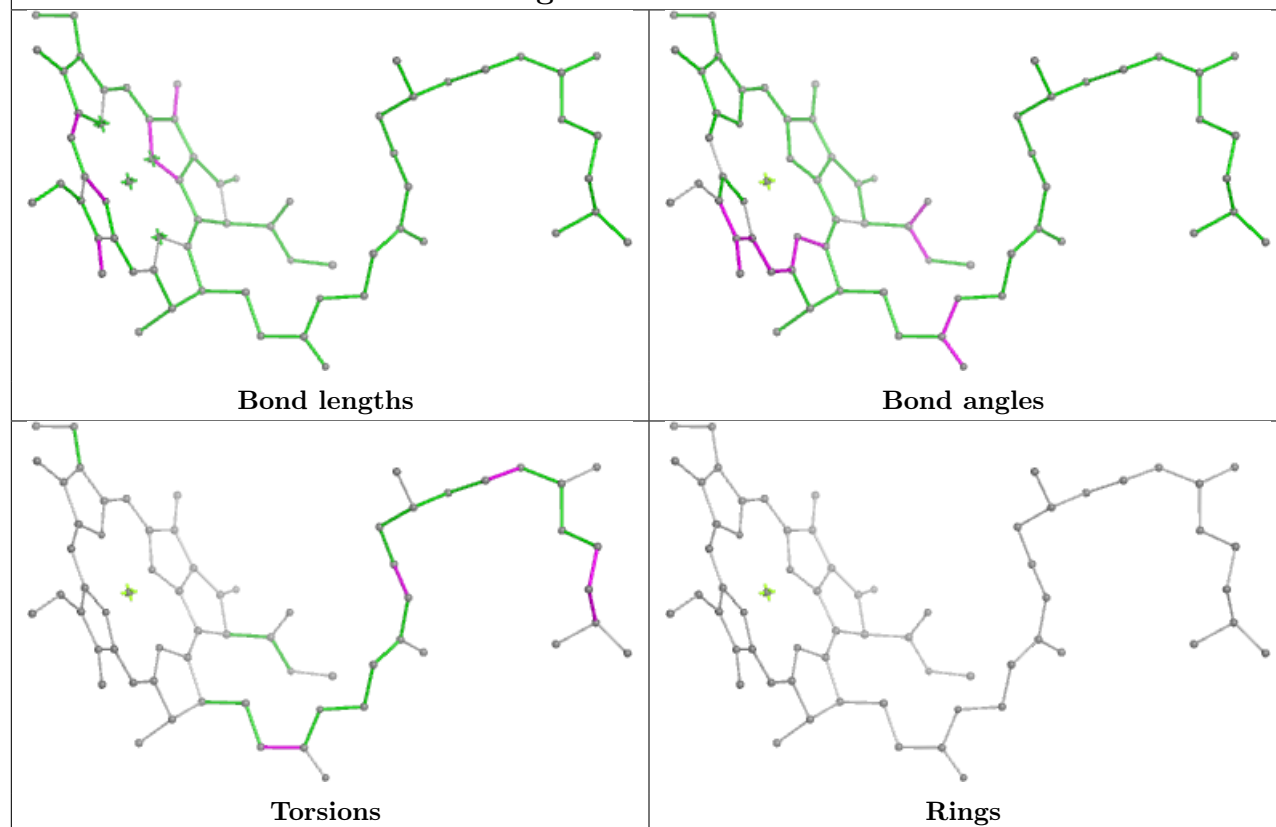




## Ligand CLA b 824

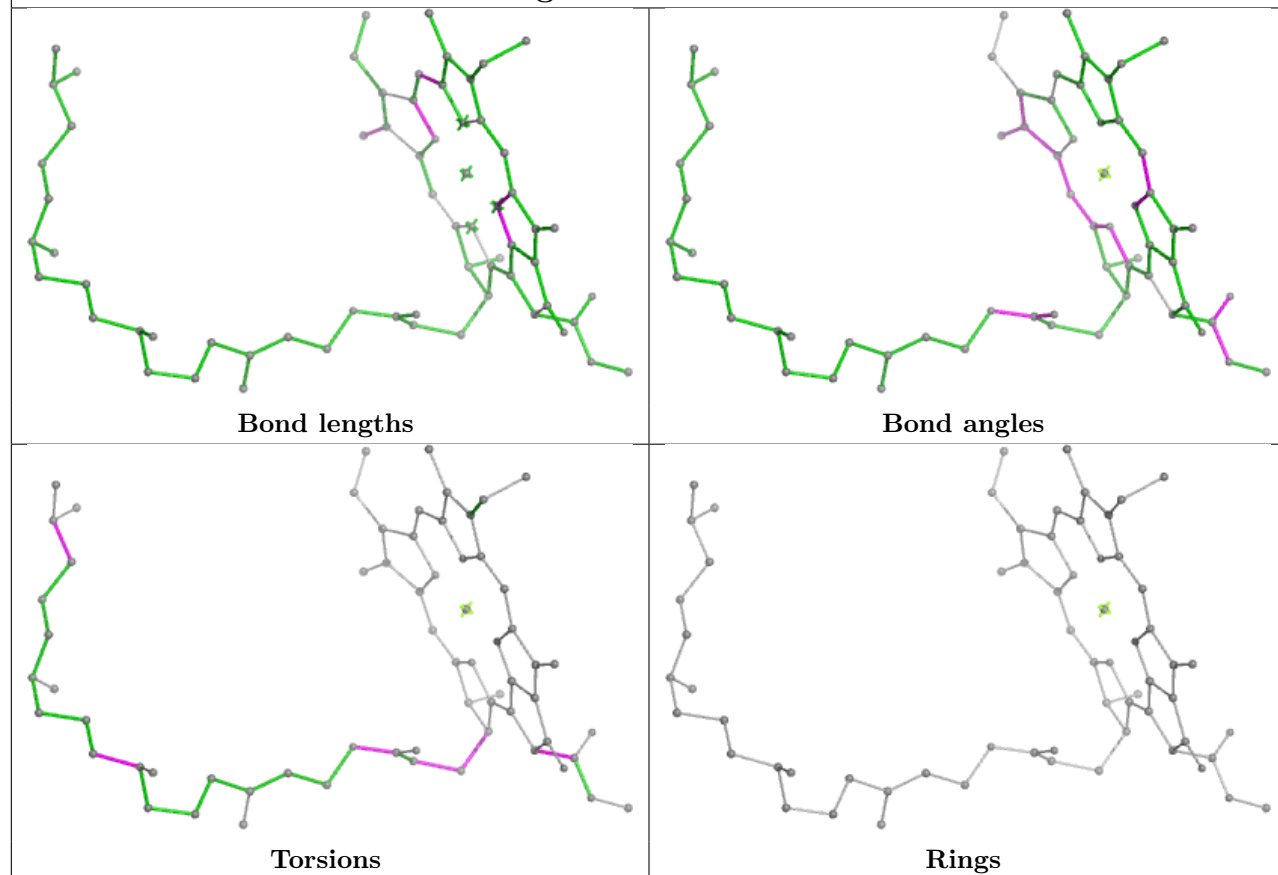


## Ligand CL0 A 801

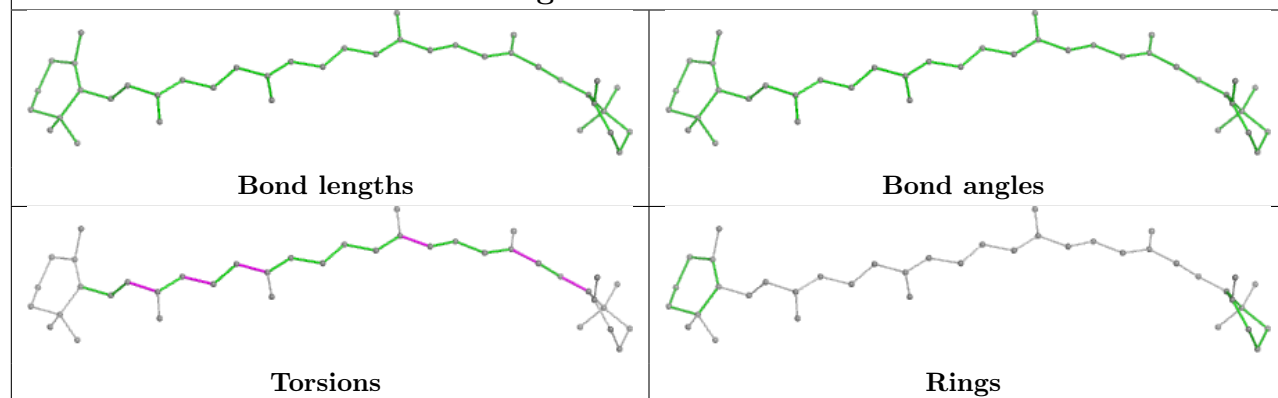




## Ligand CLA a 842

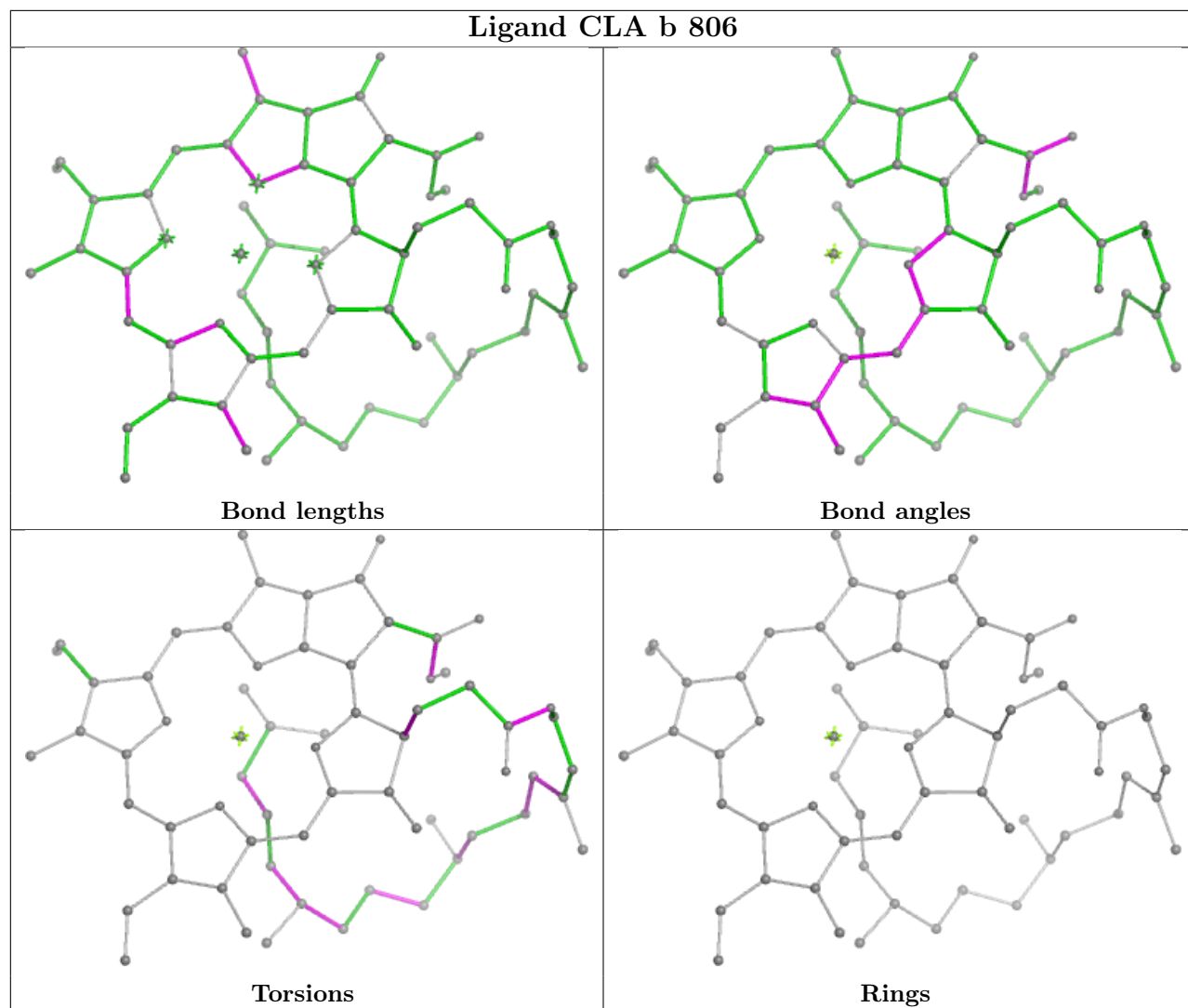


## Ligand BCR I 101

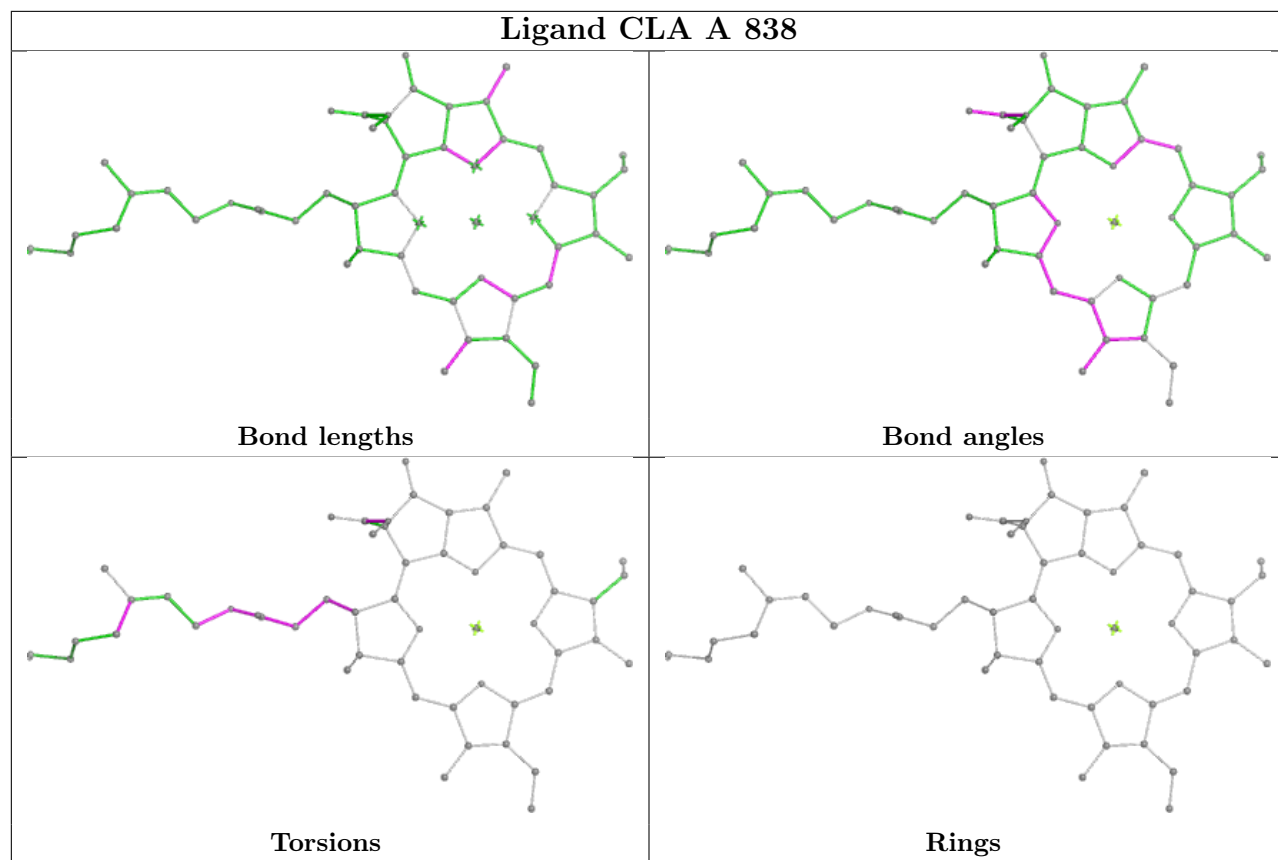




## Ligand CLA b 806

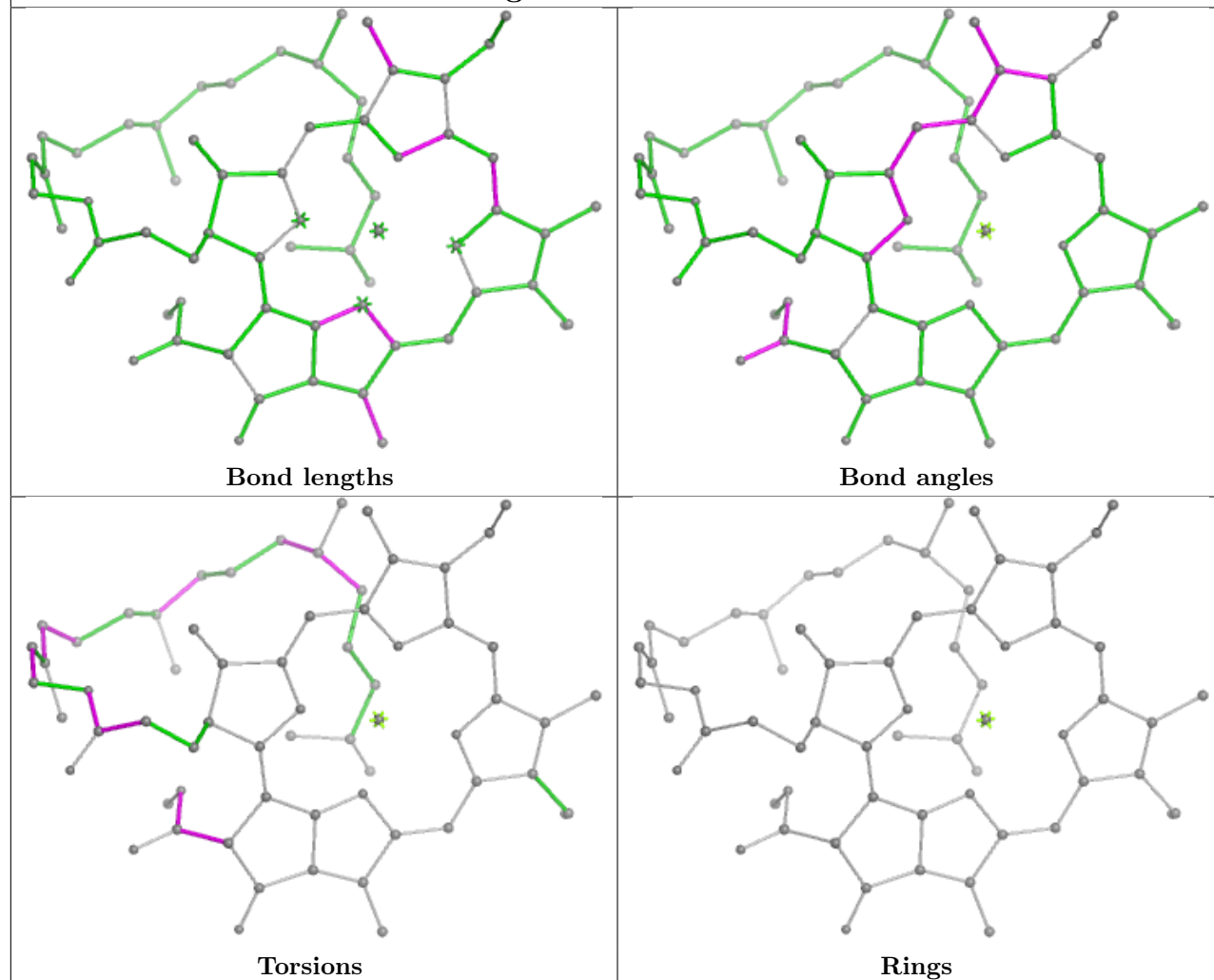




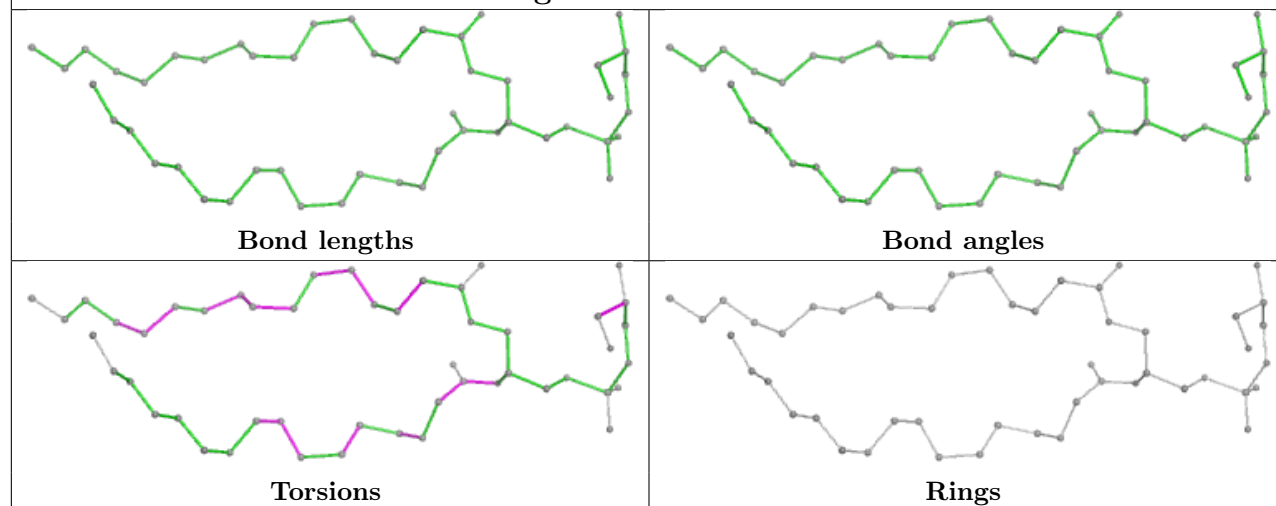




## Ligand CLA A 807

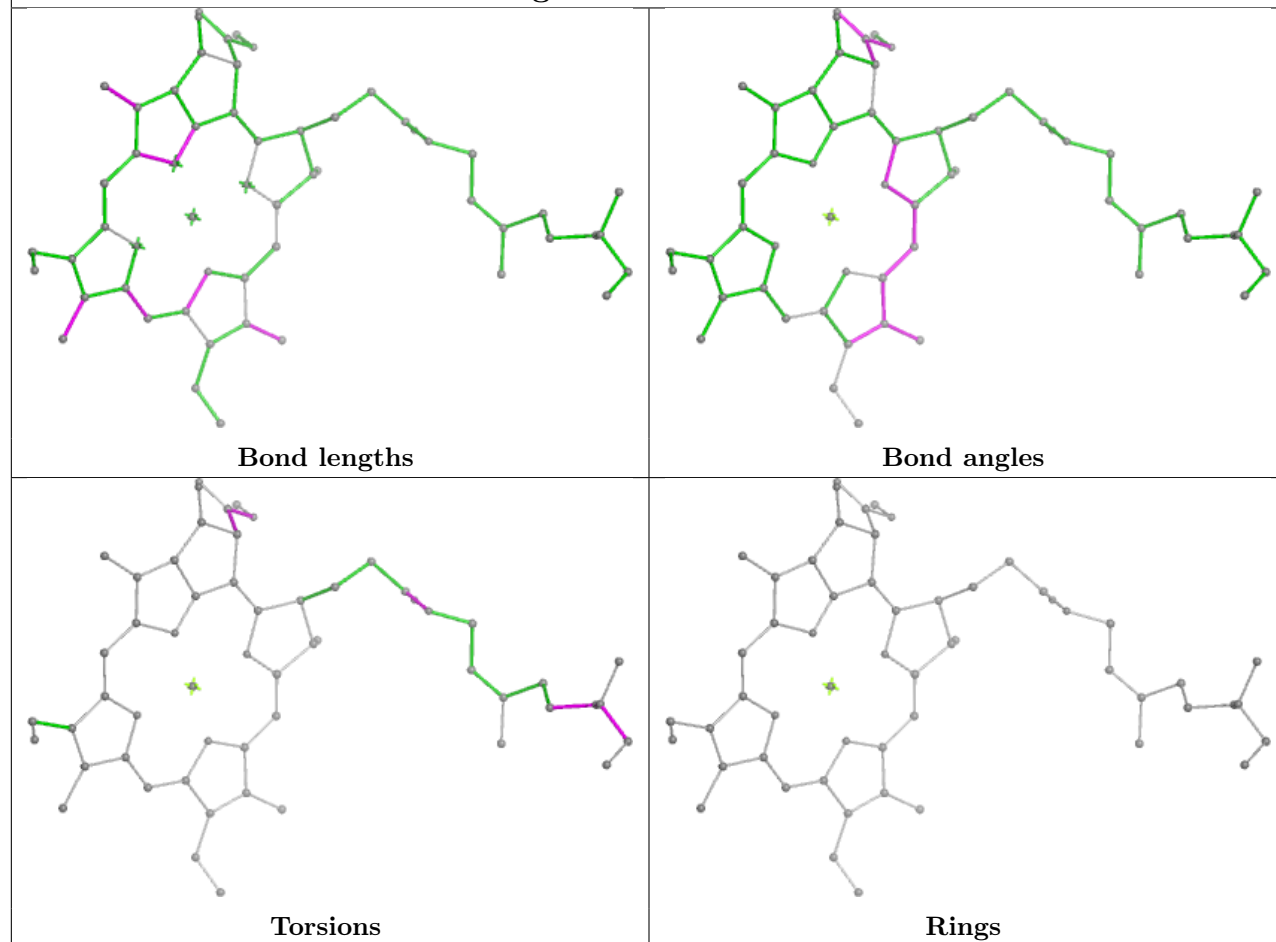


## Ligand LHG k 101

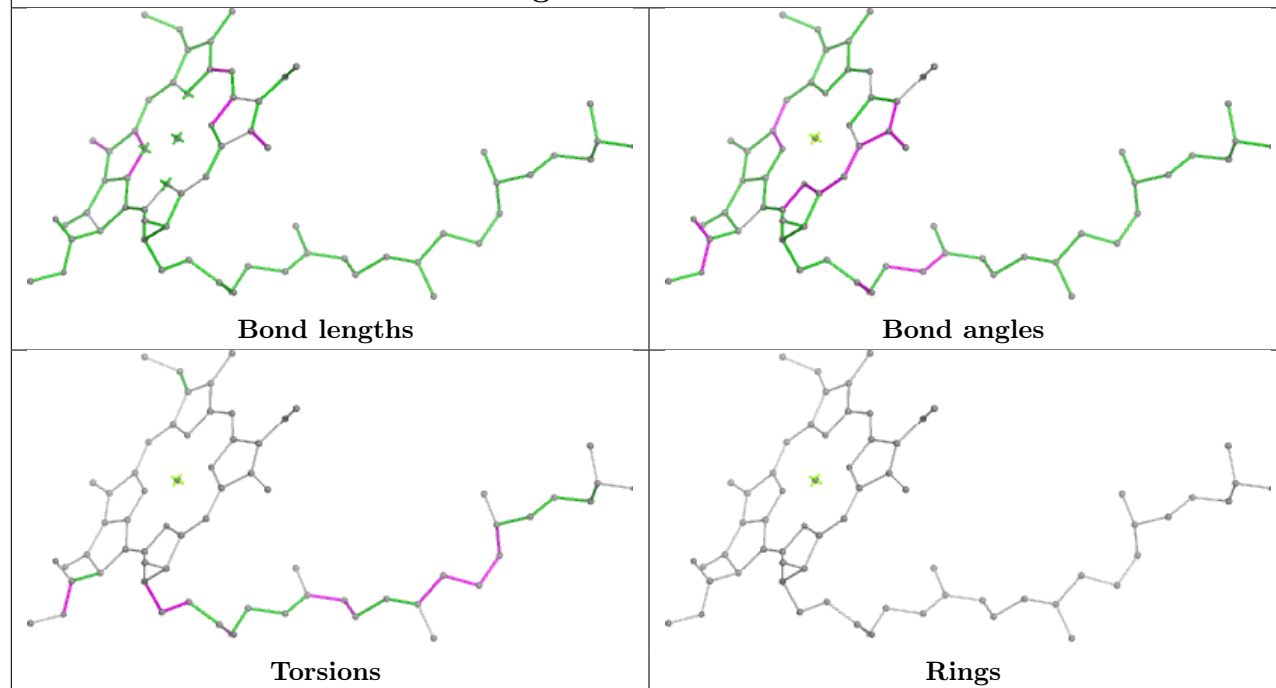




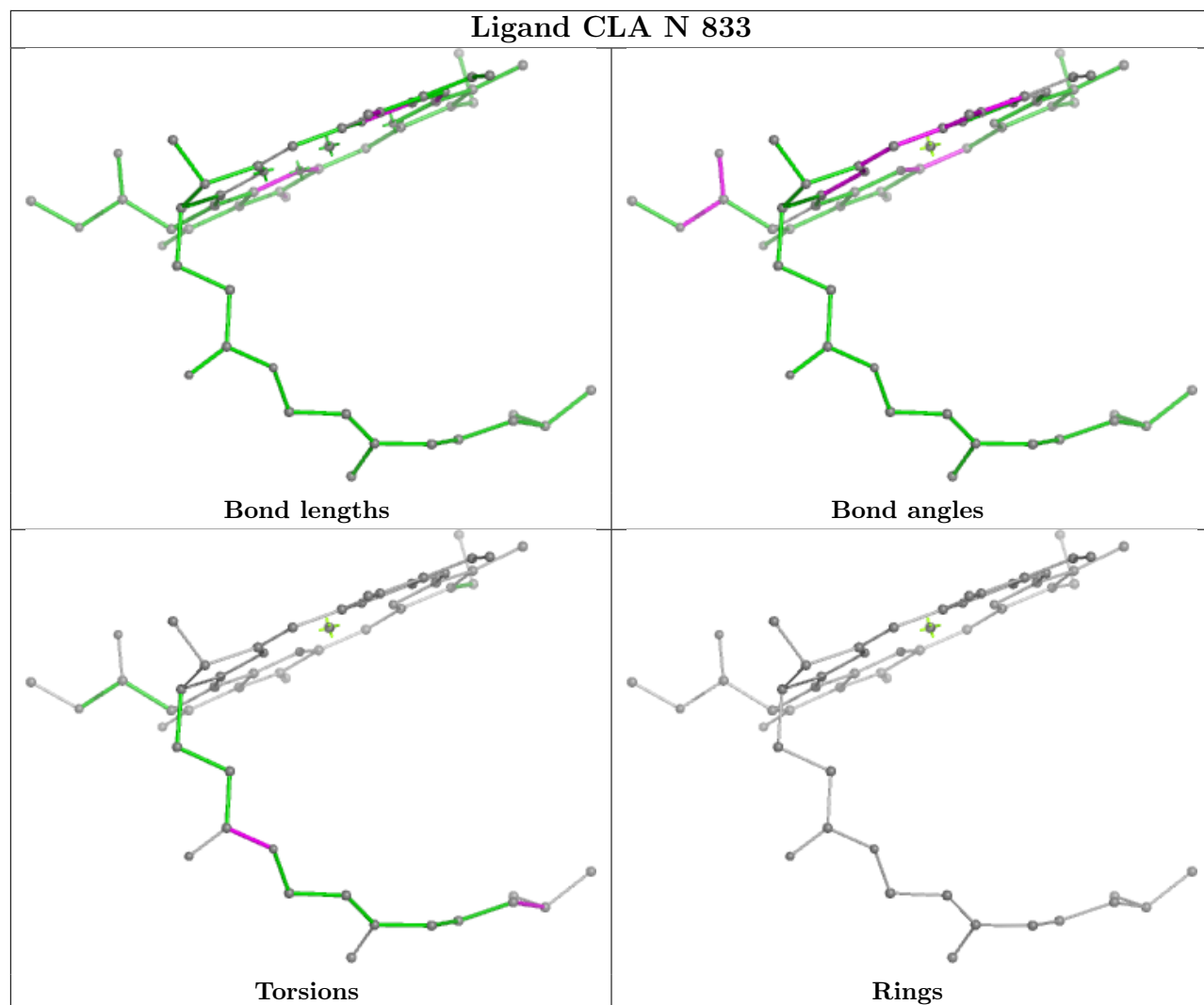
## Ligand CLA B 811



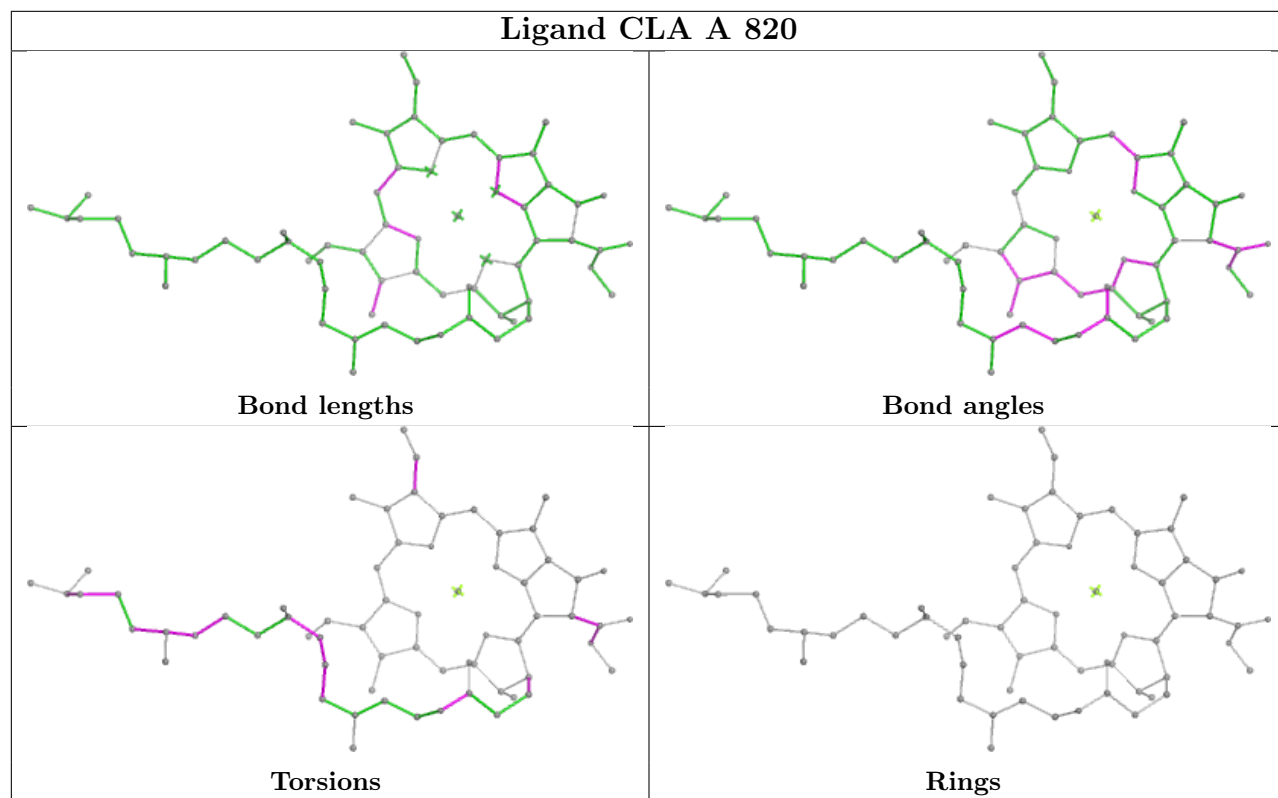
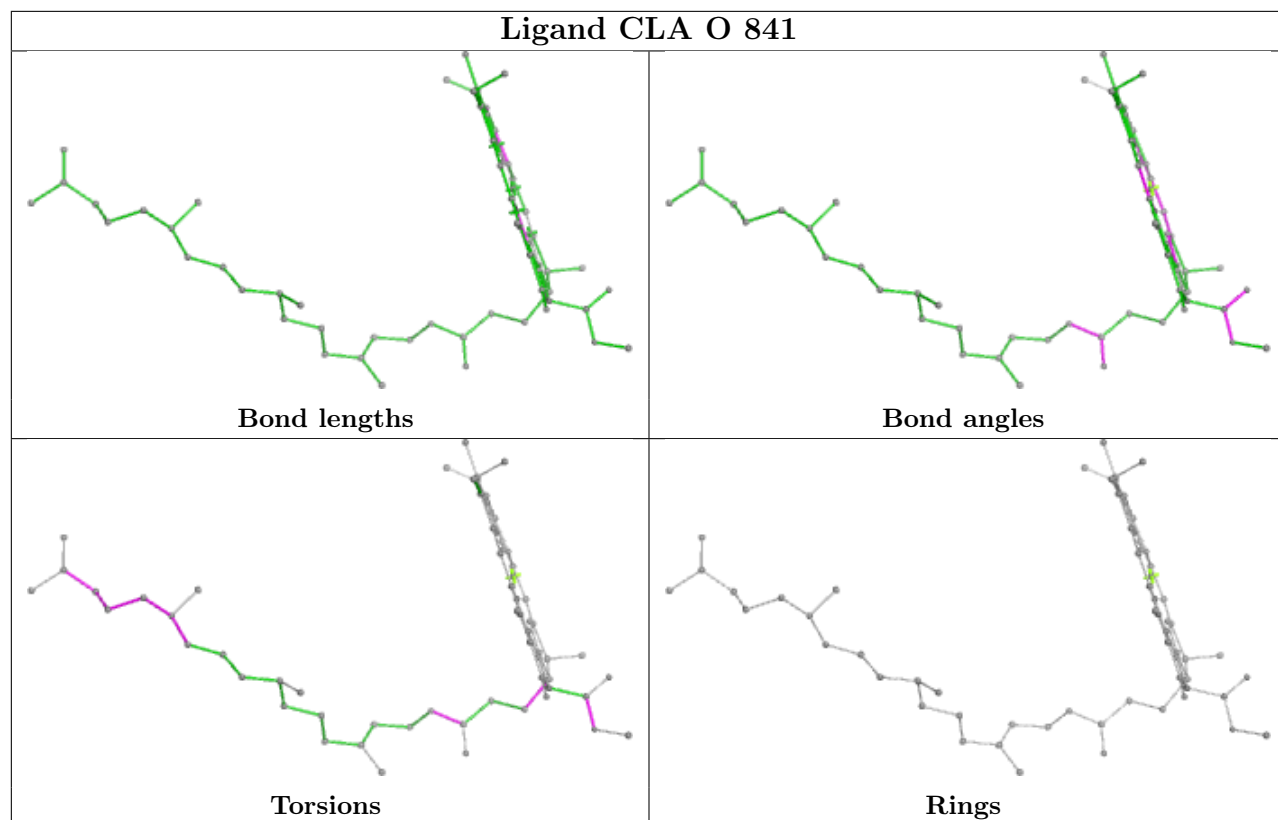
## Ligand CLA B 829



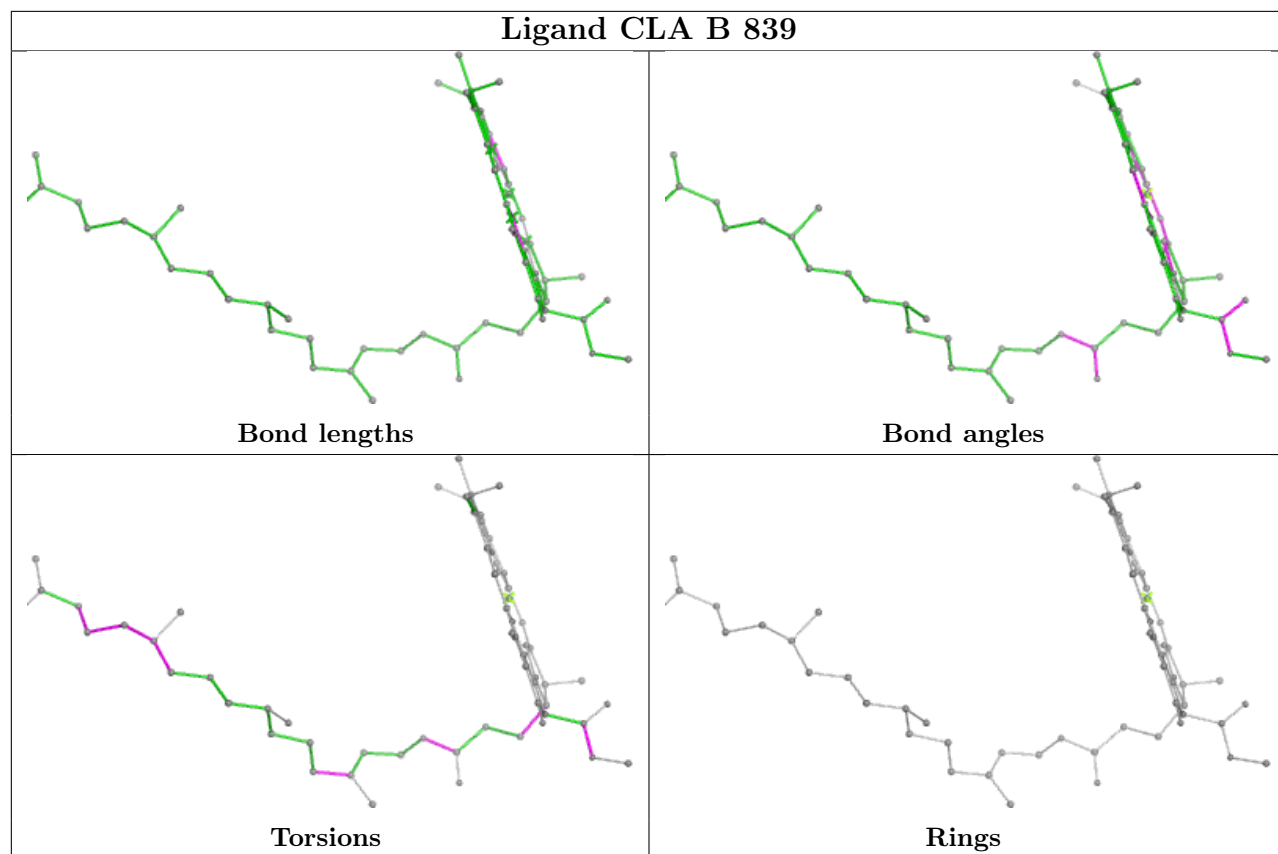




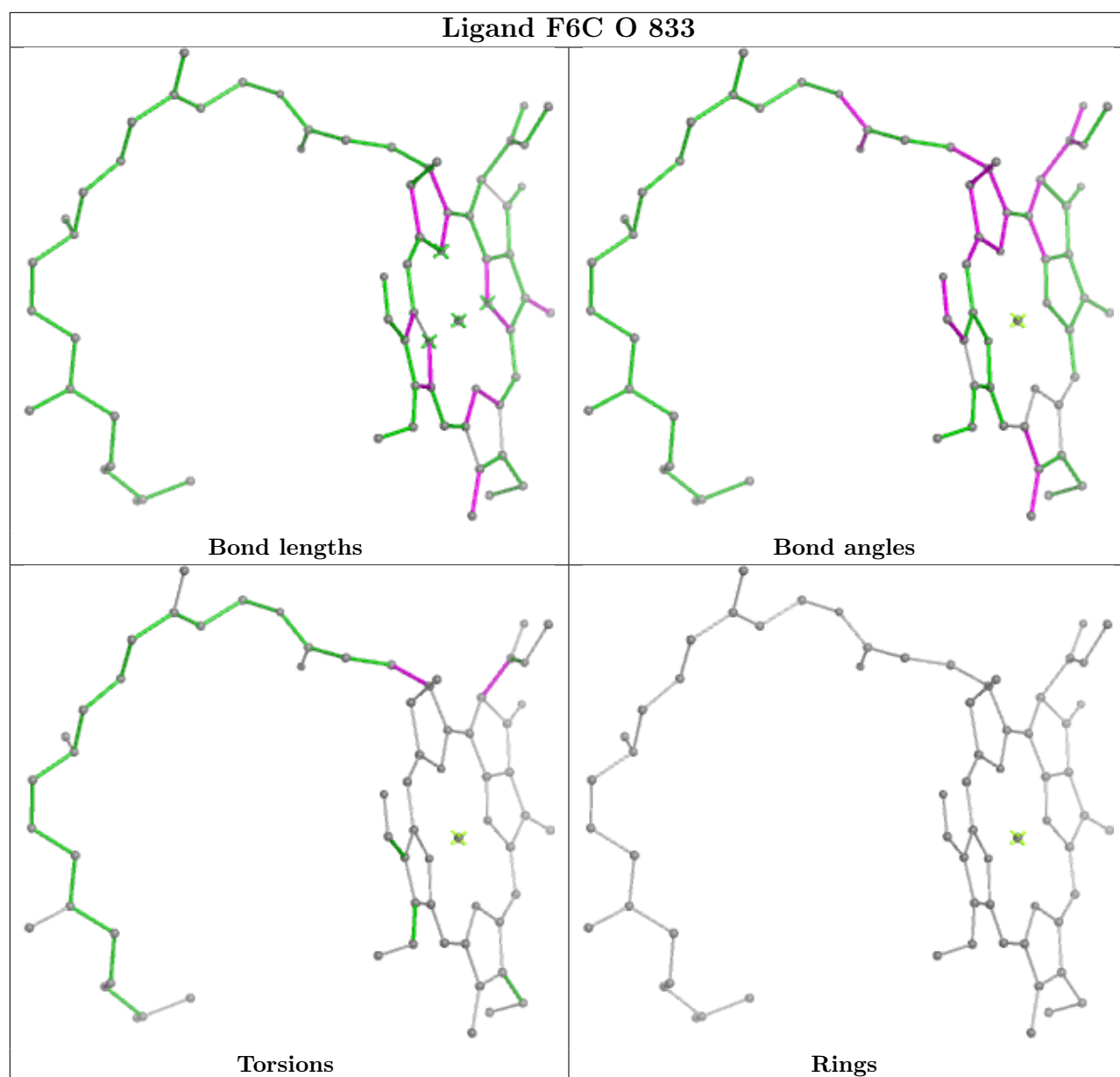




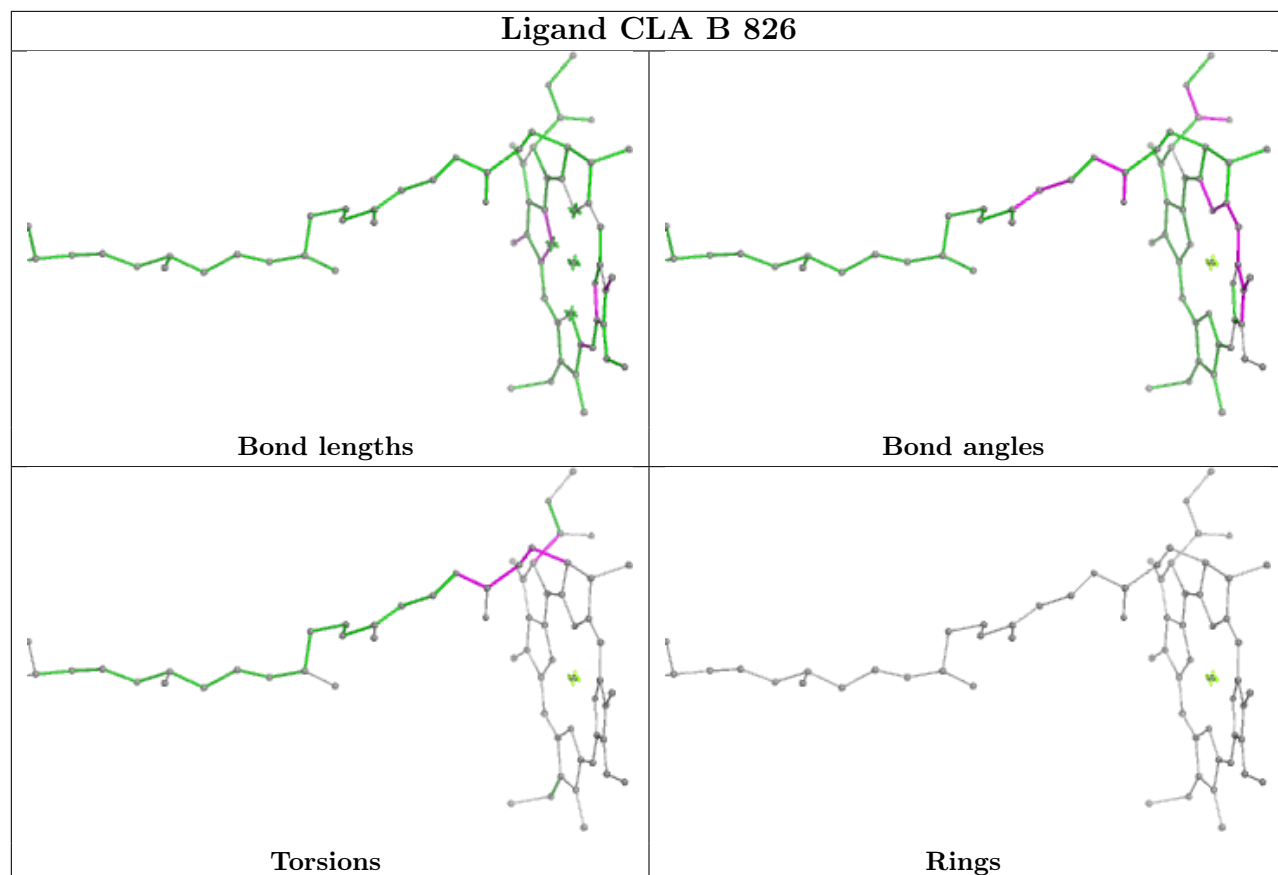
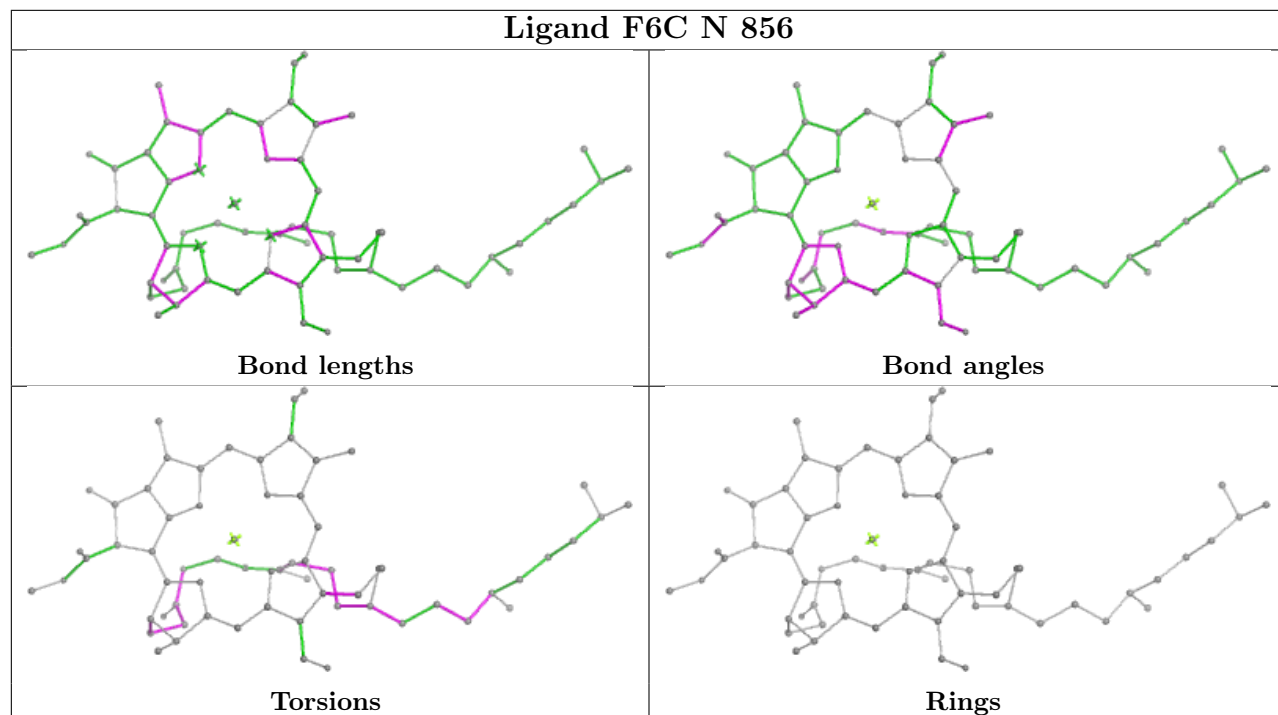




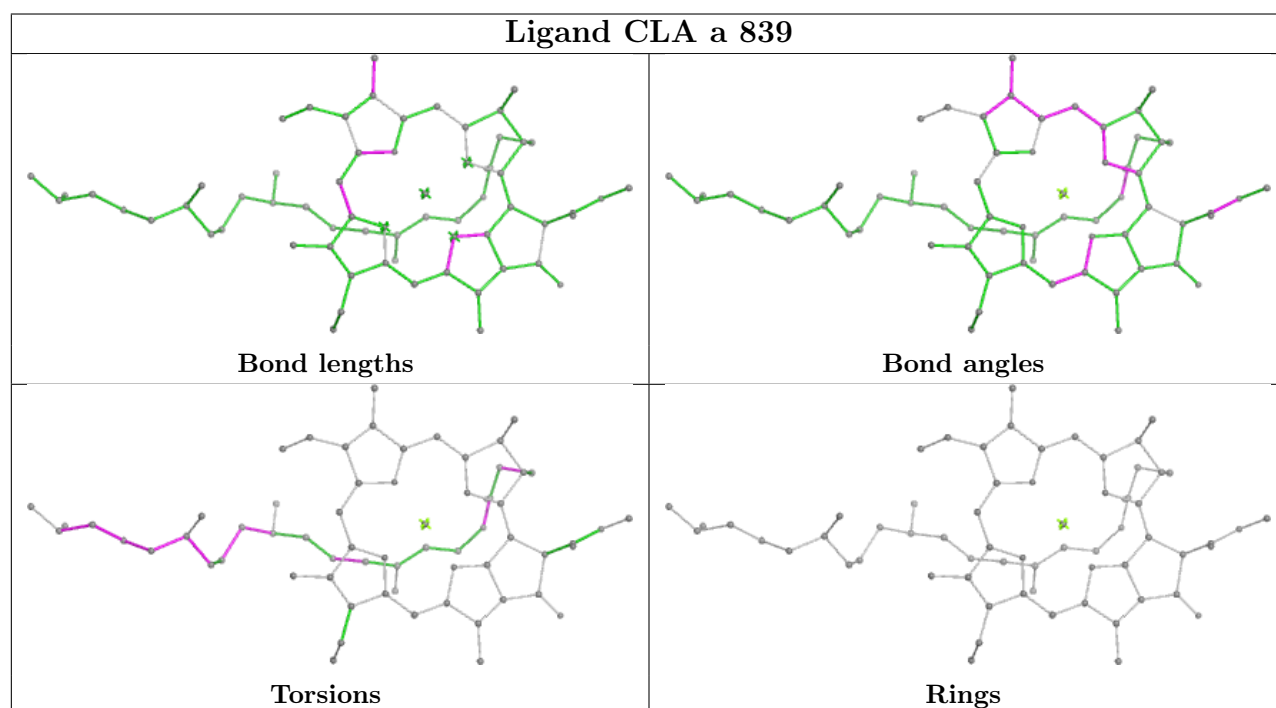
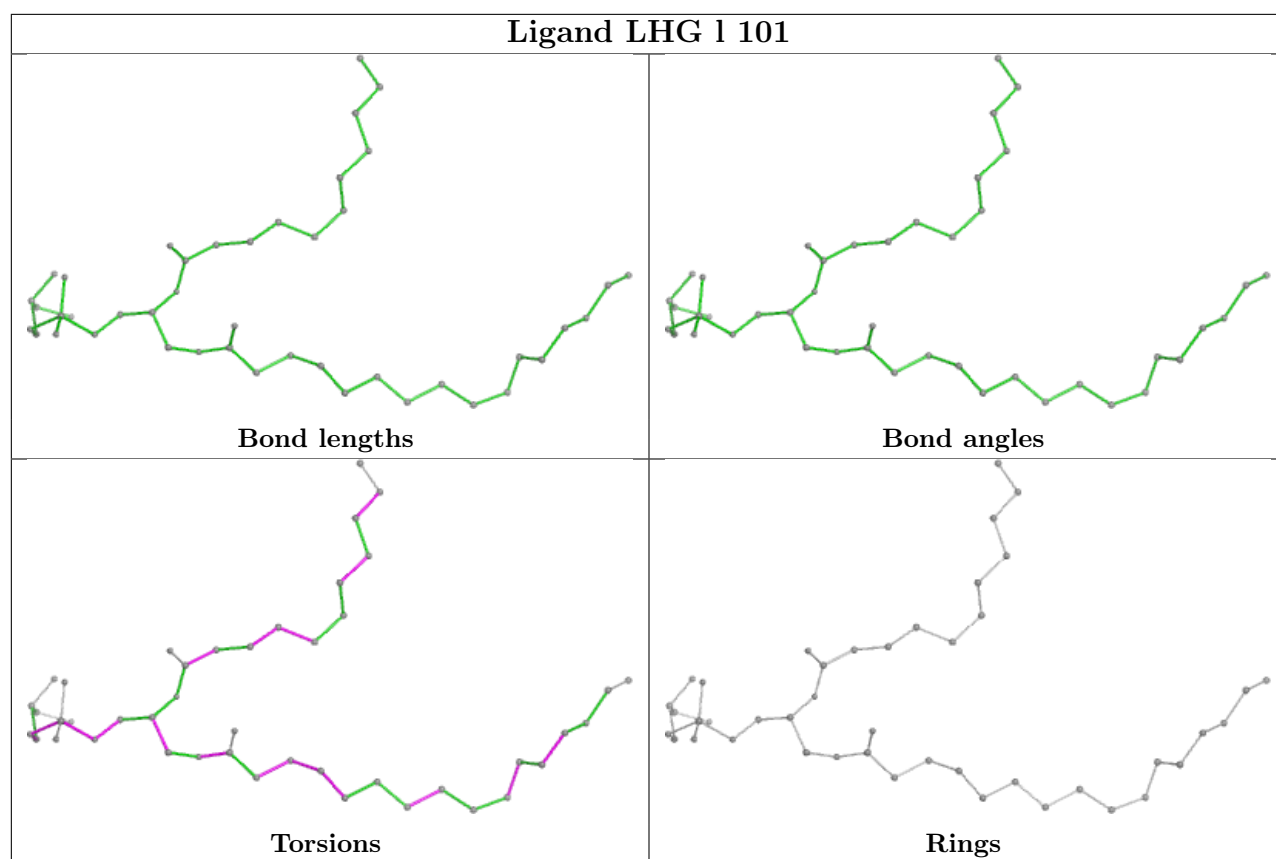






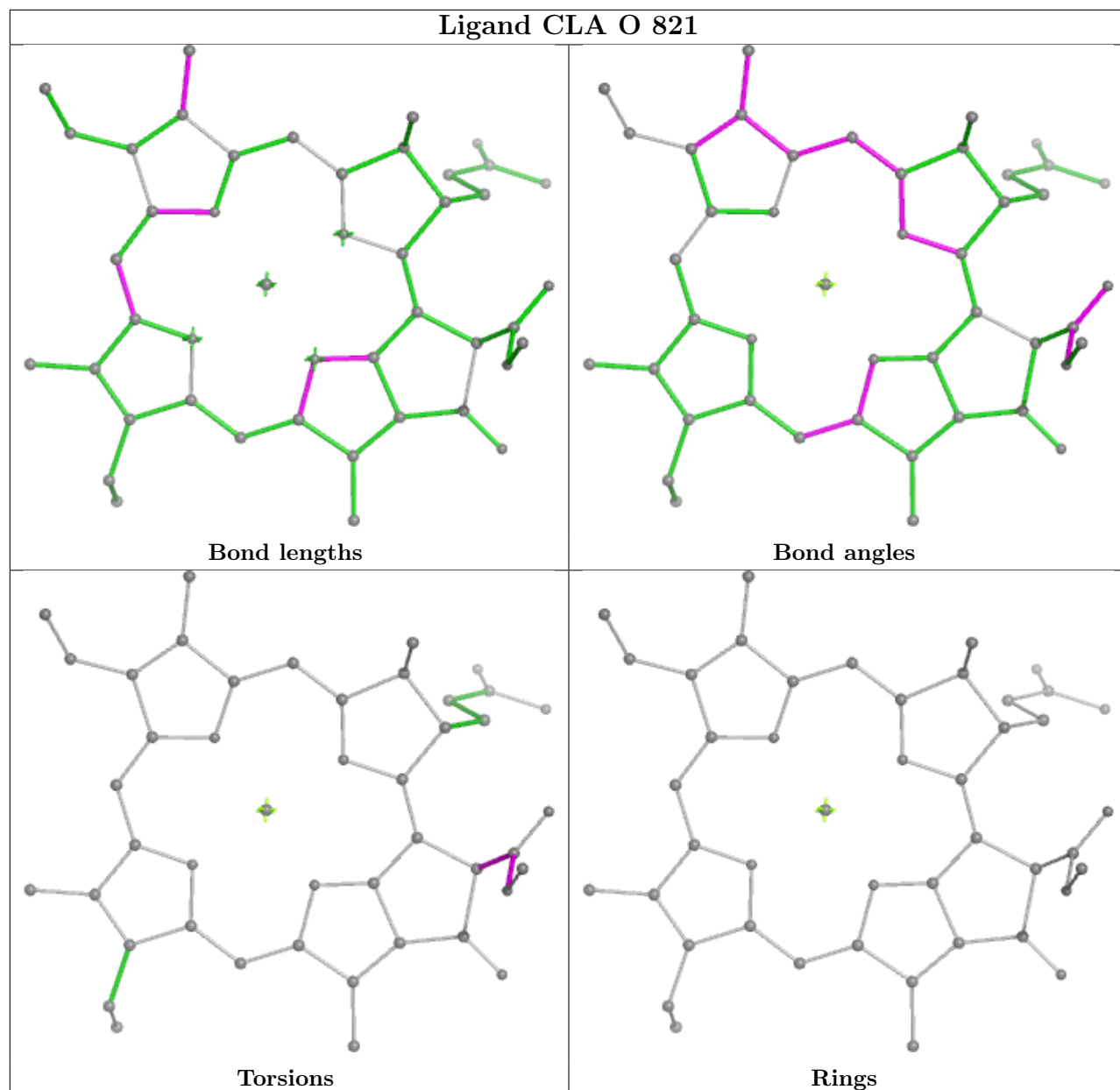
**Ligand CLA B 826****Ligand F6C N 856**



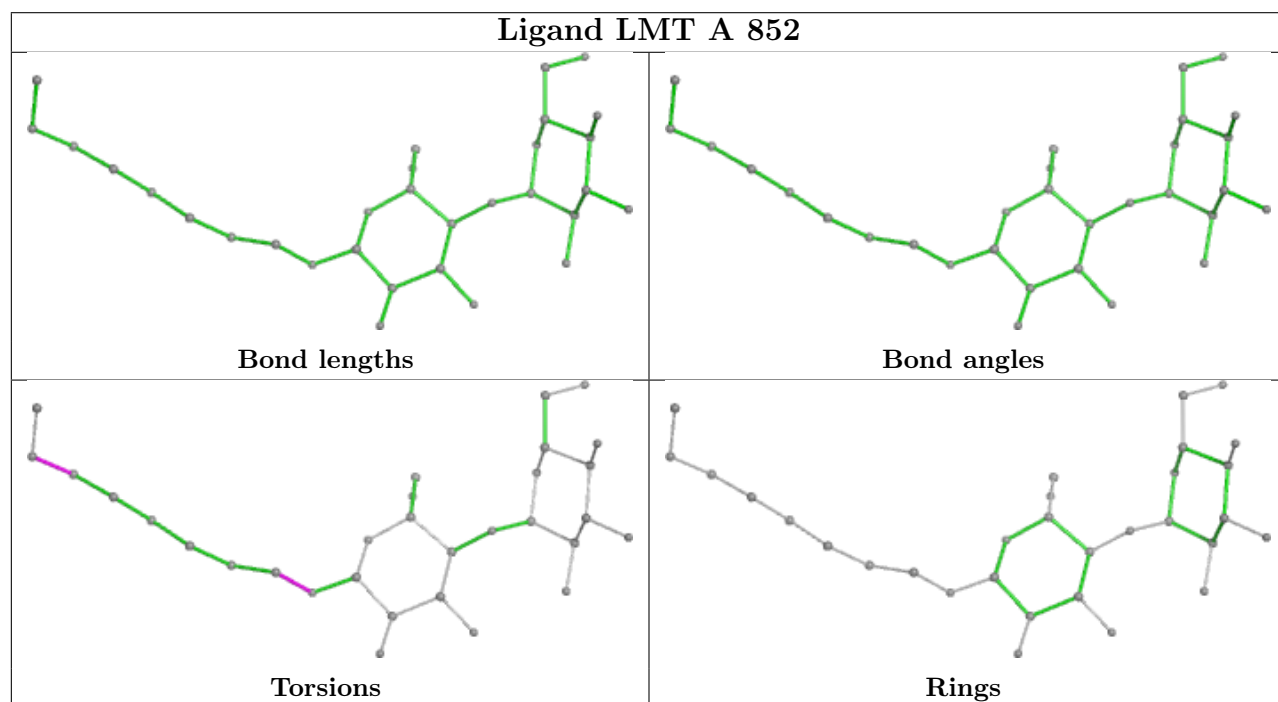
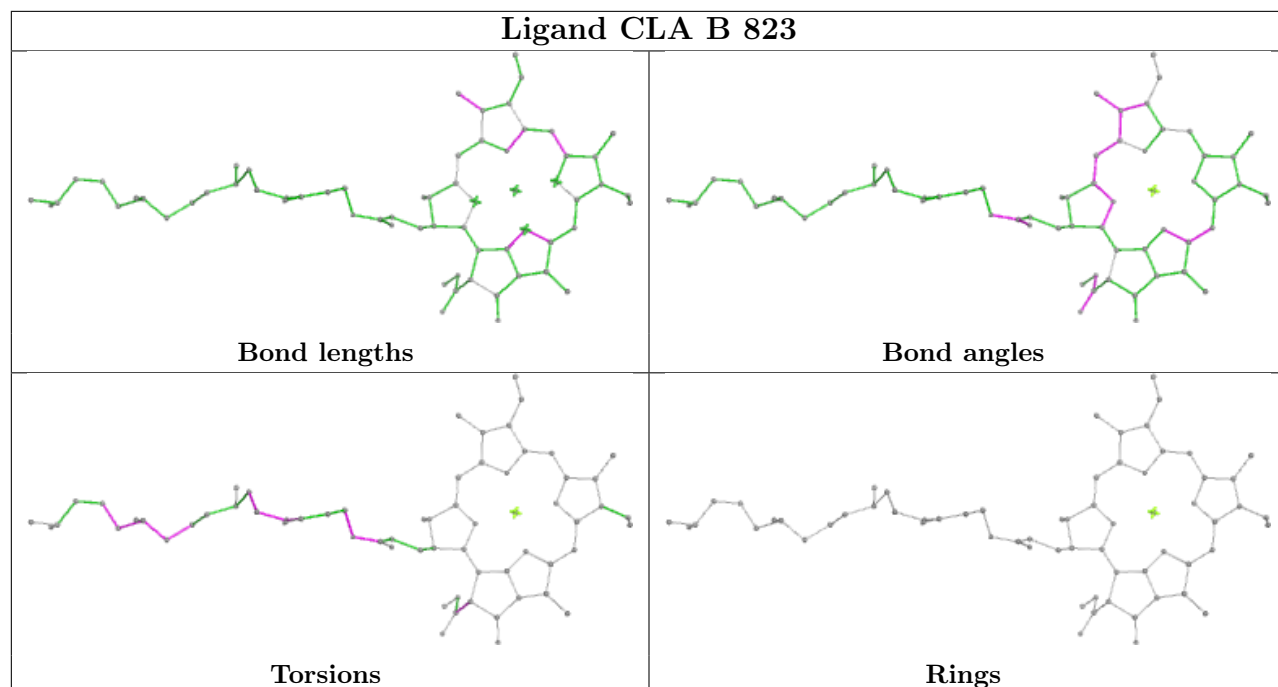




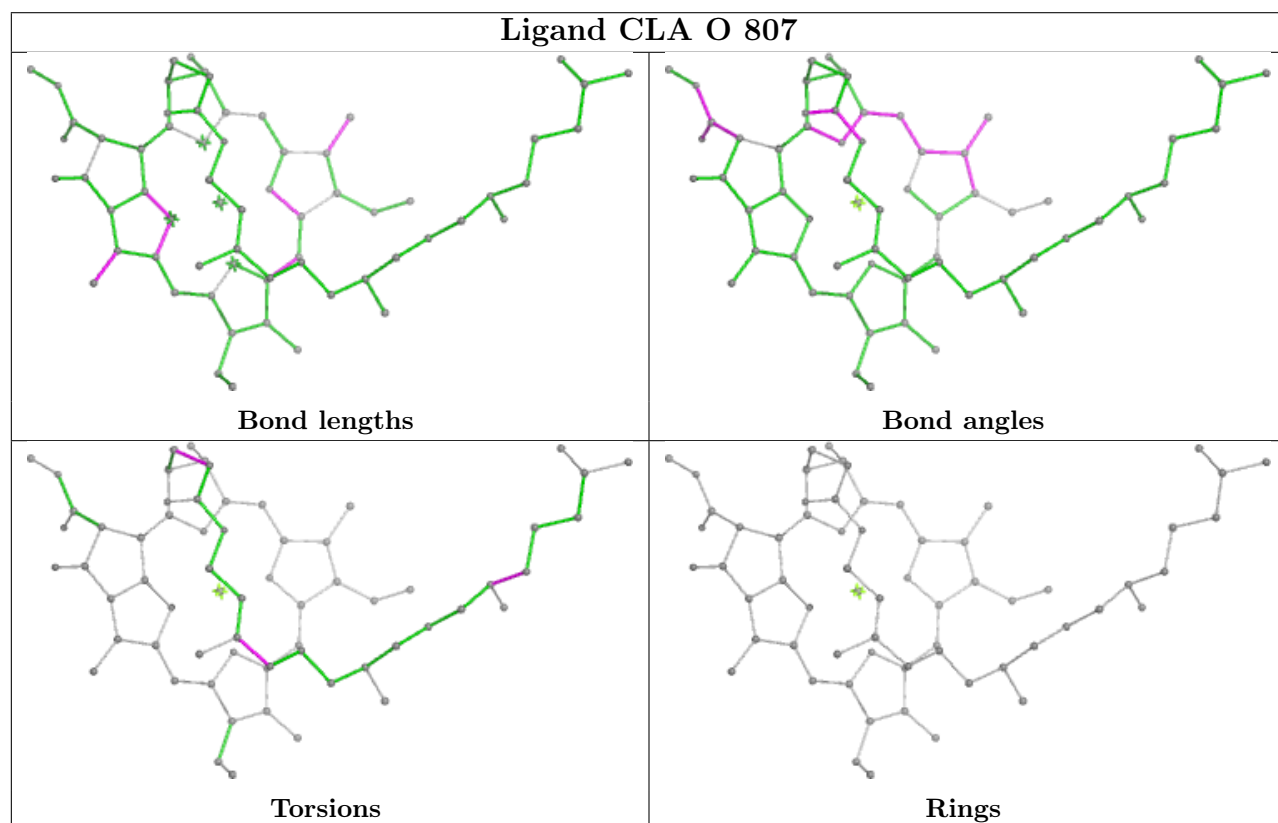
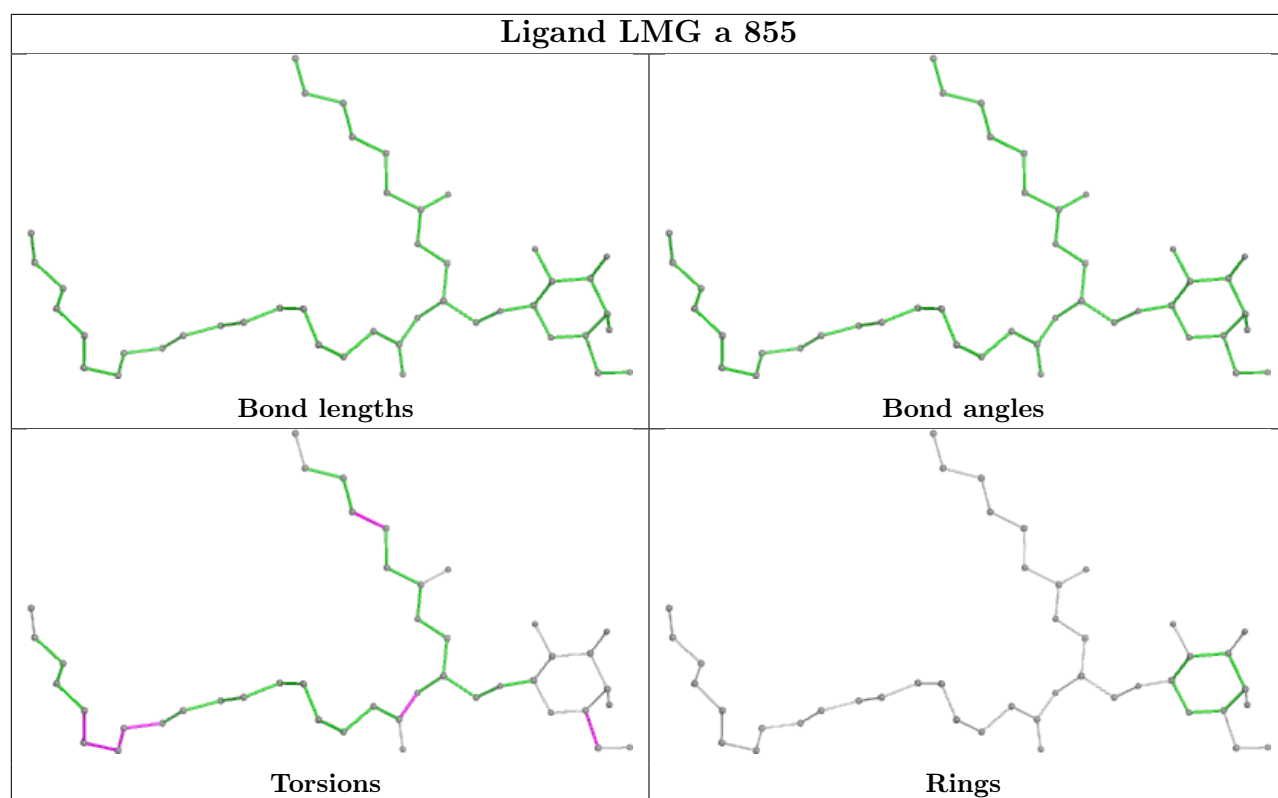
## Ligand CLA O 821





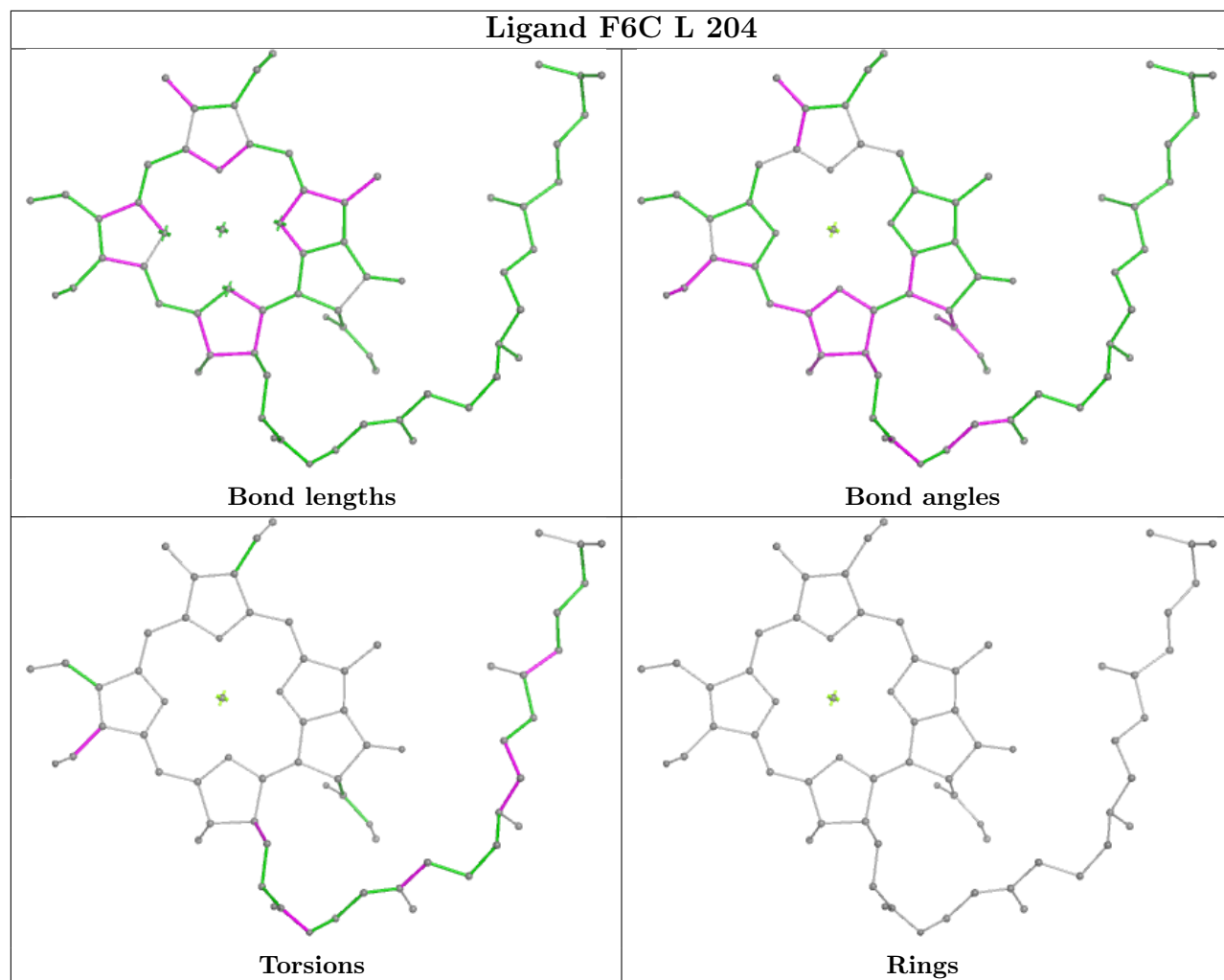




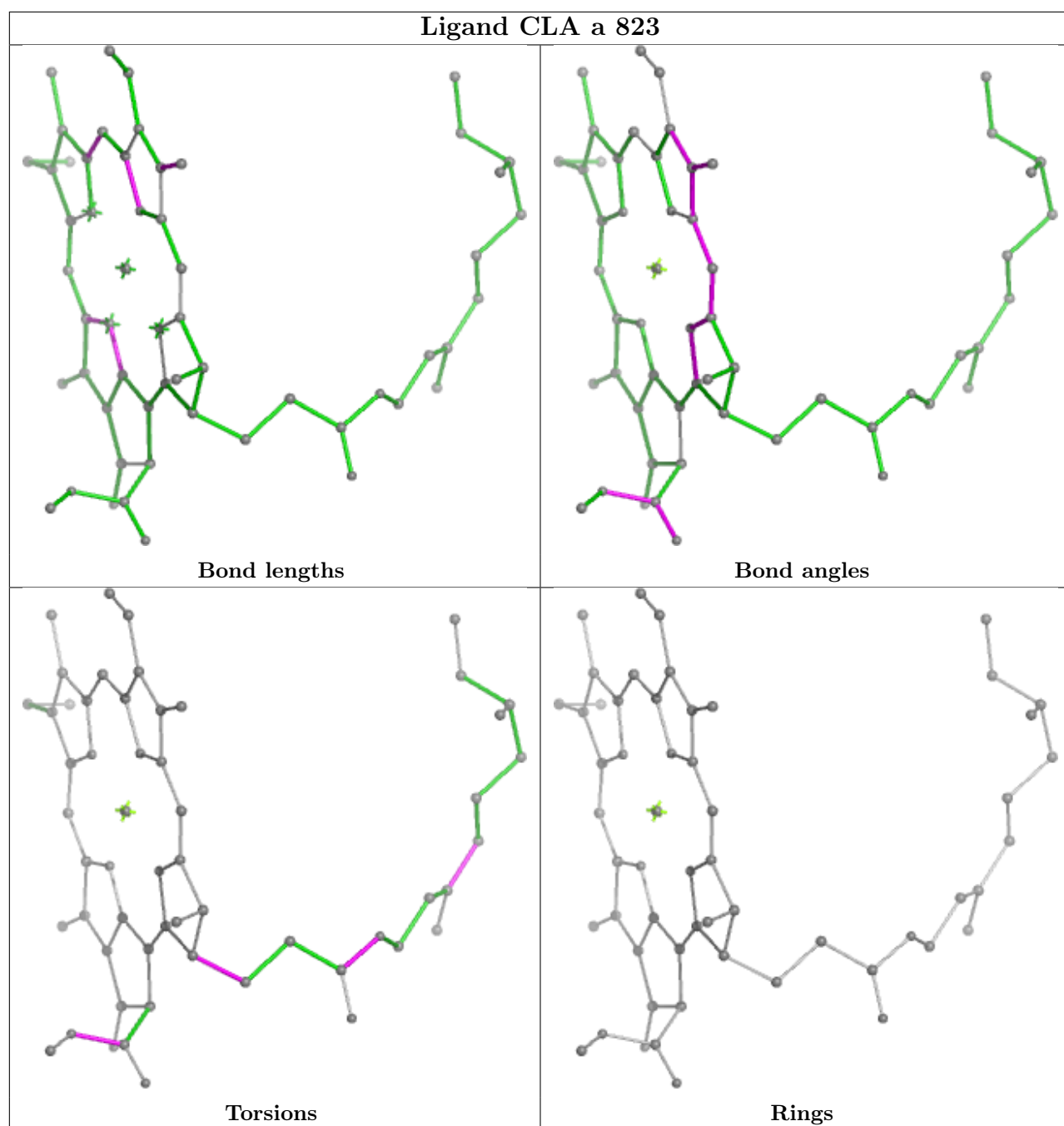




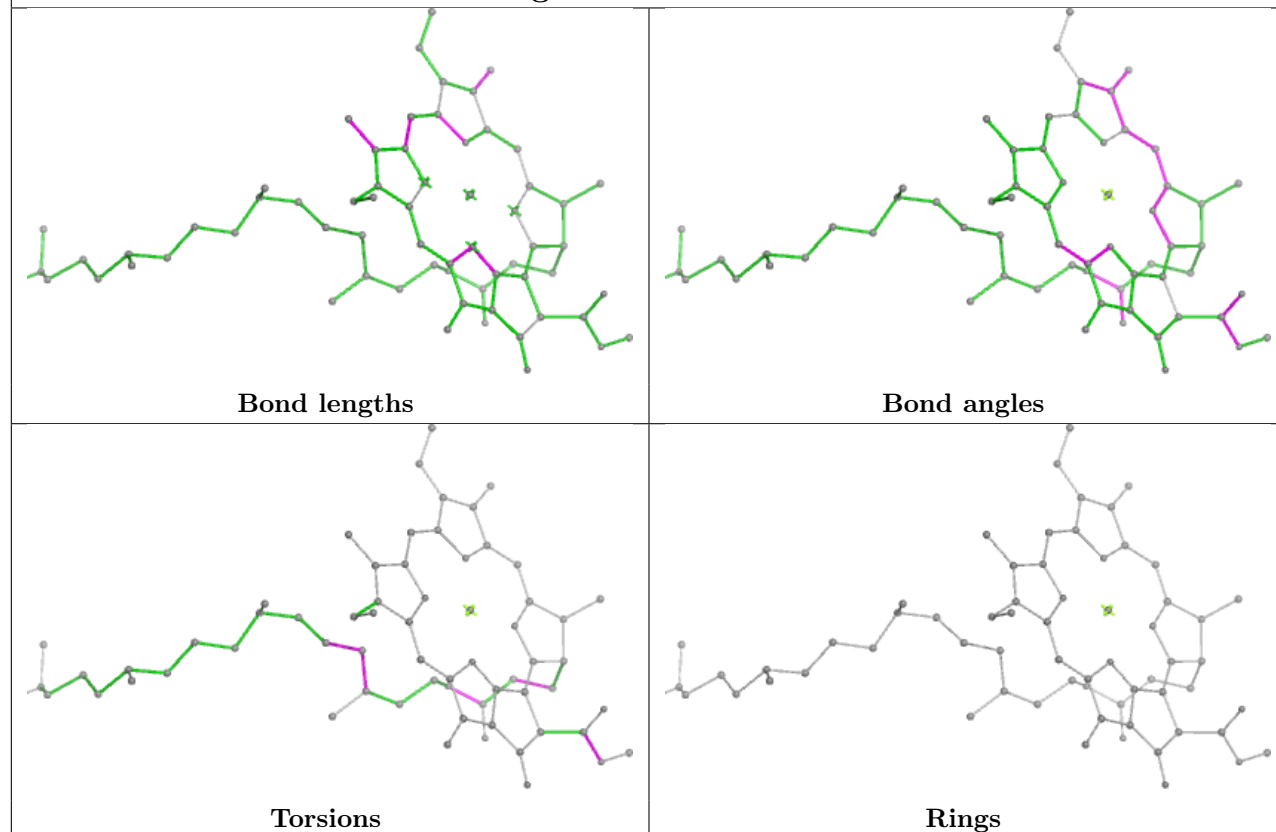
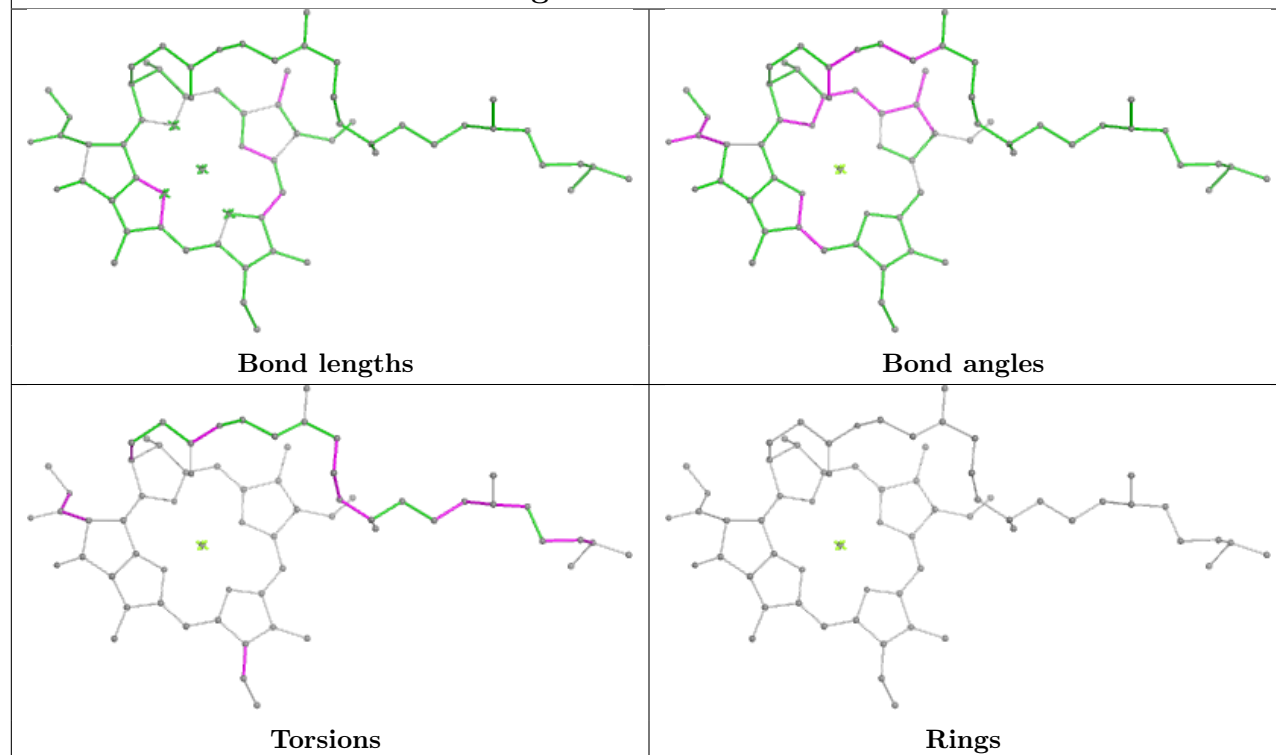
## Ligand F6C L 204



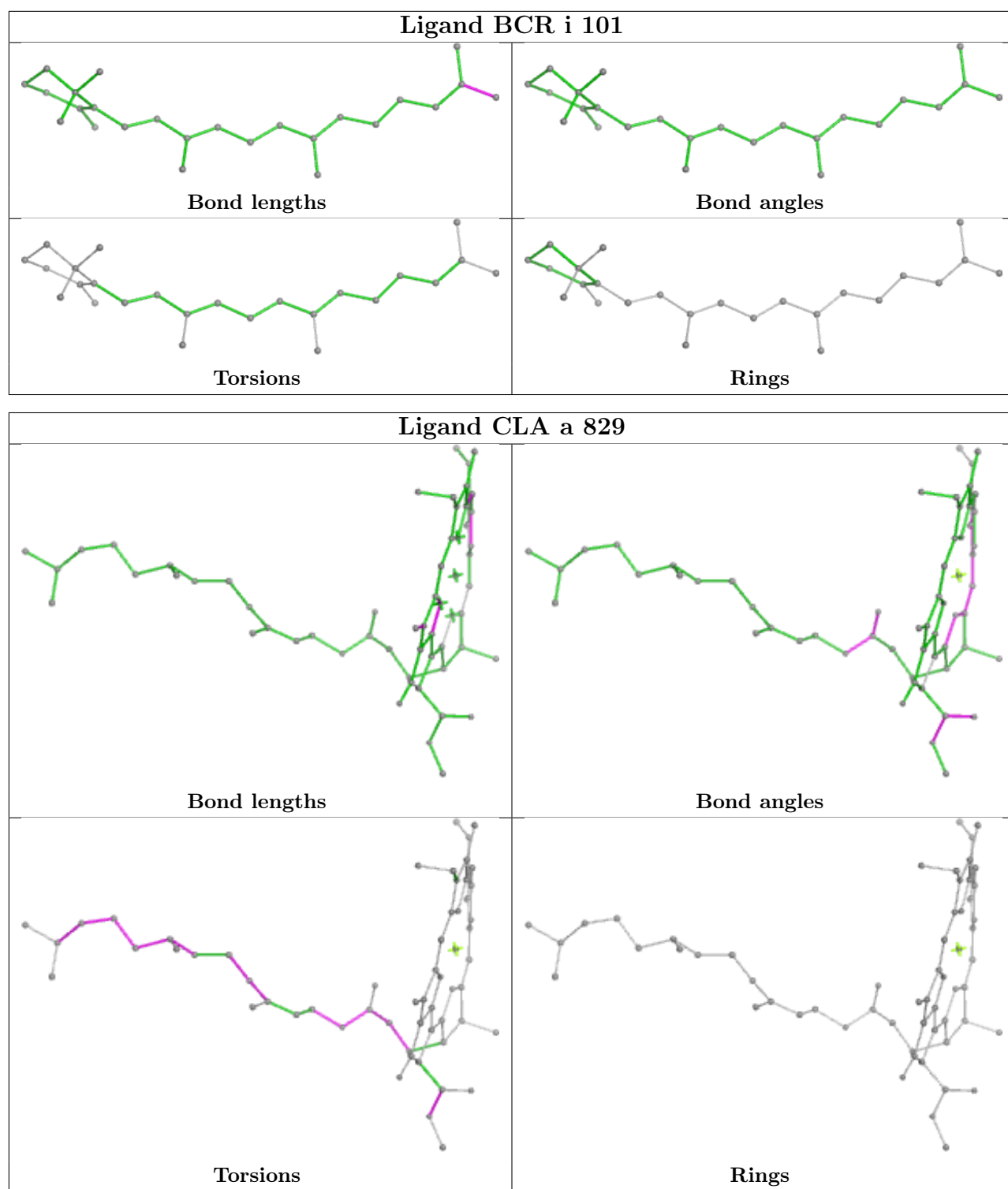




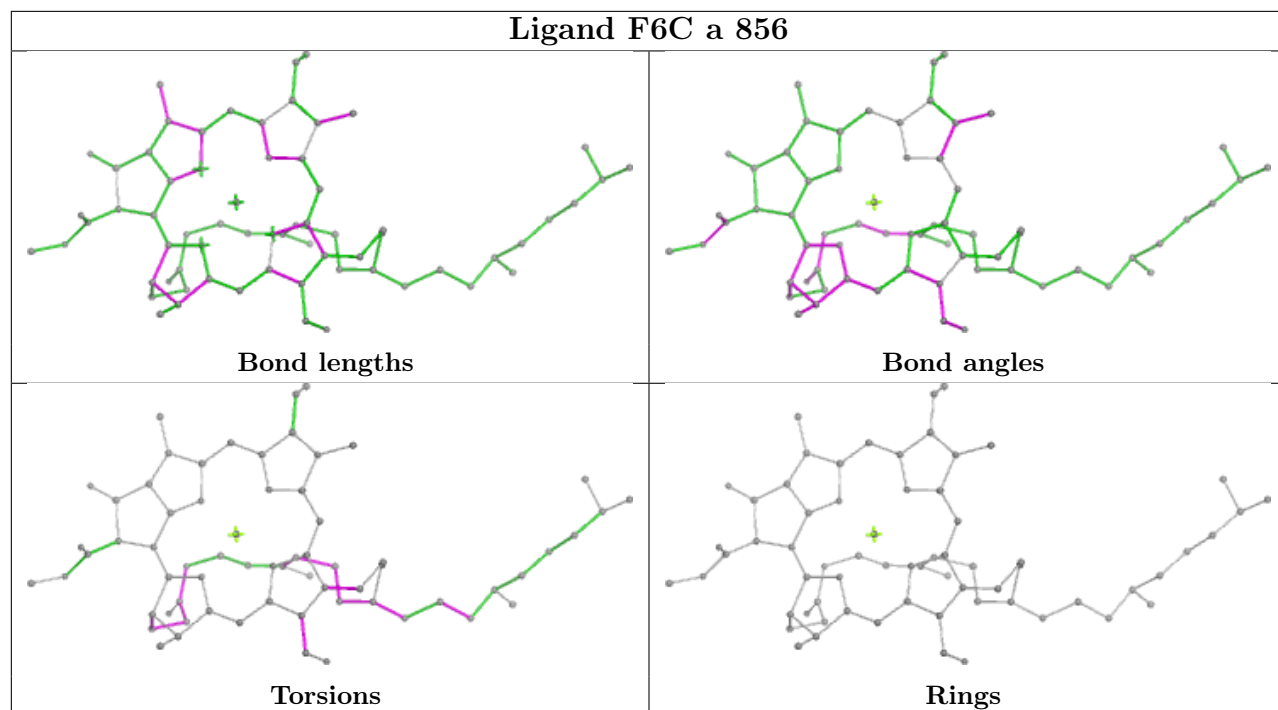
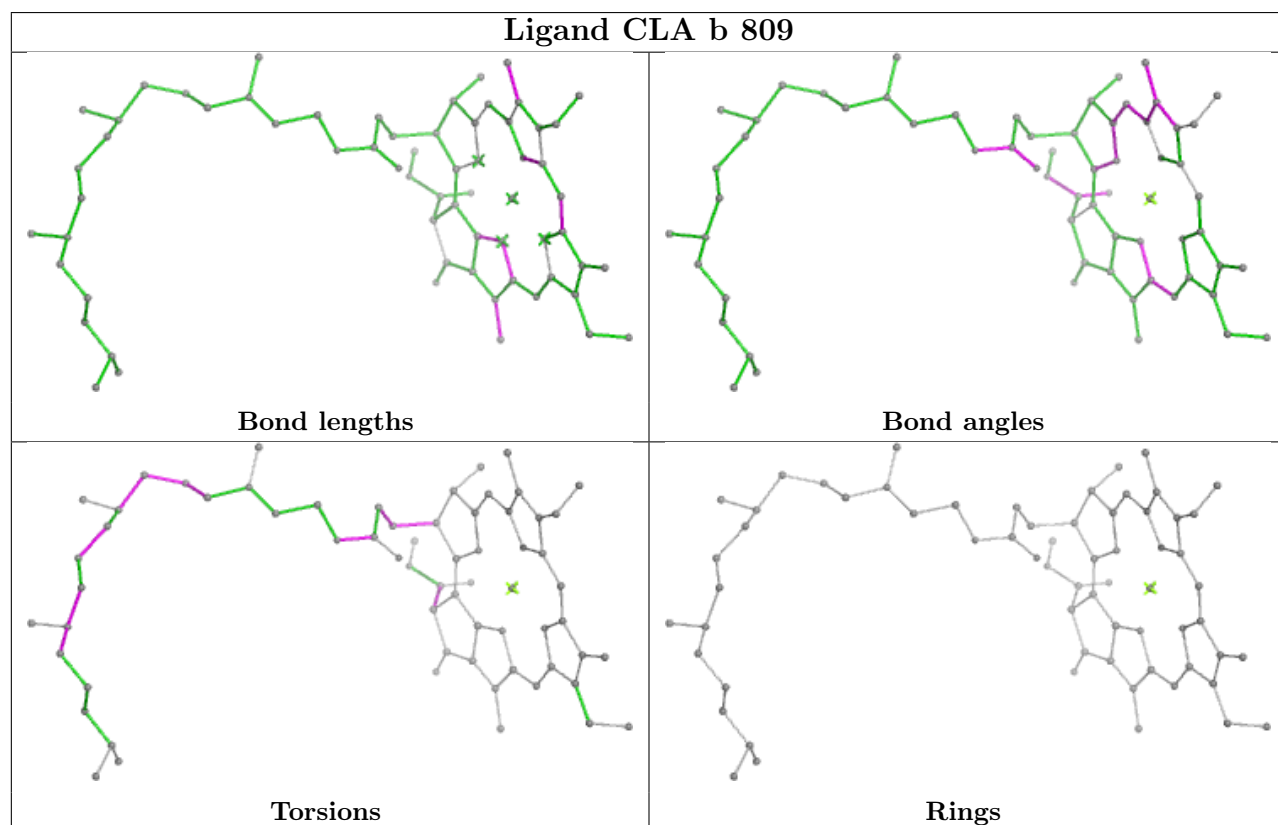


**Ligand CLA O 804****Ligand CLA N 820**

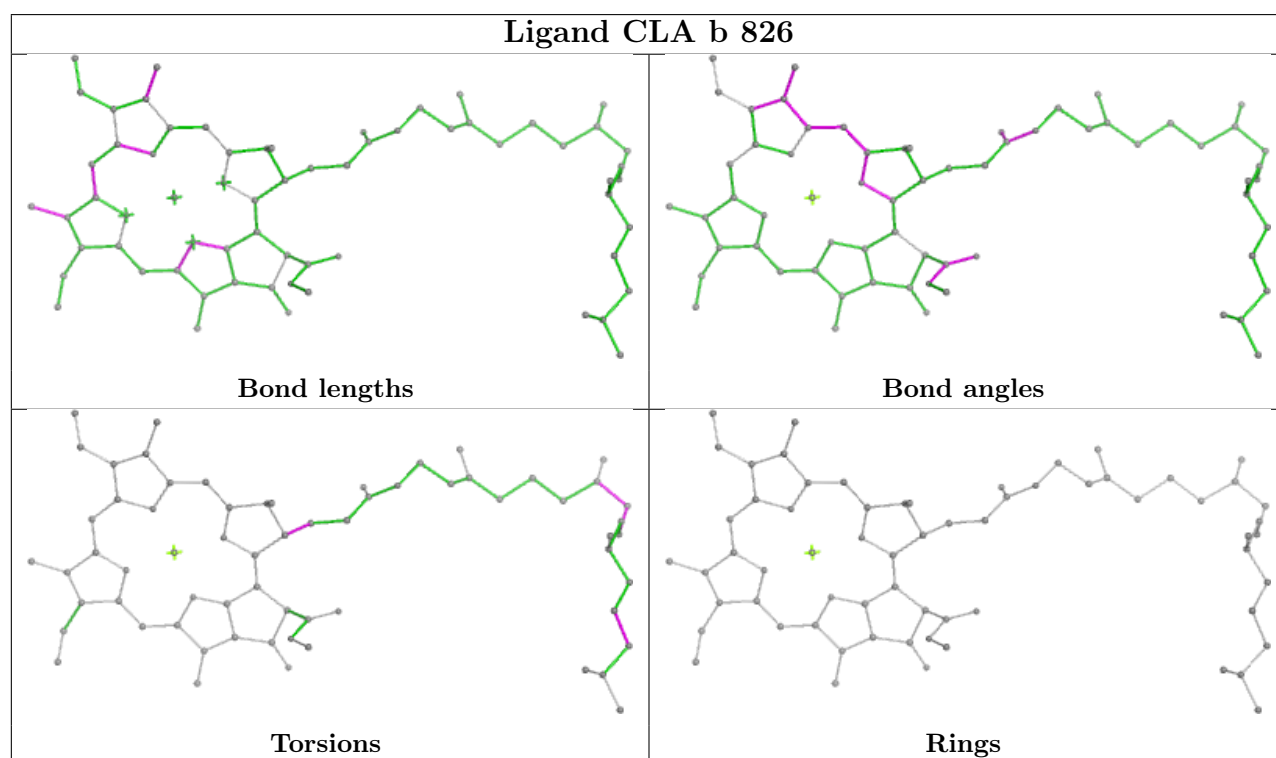
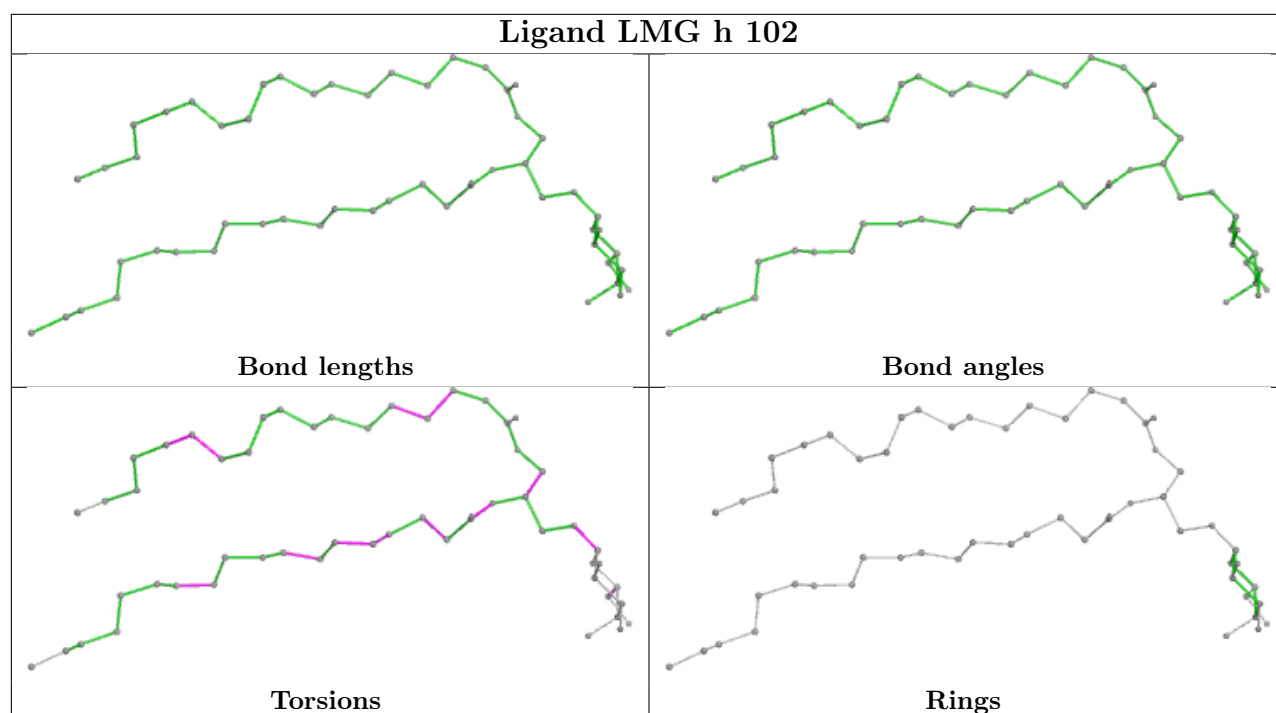




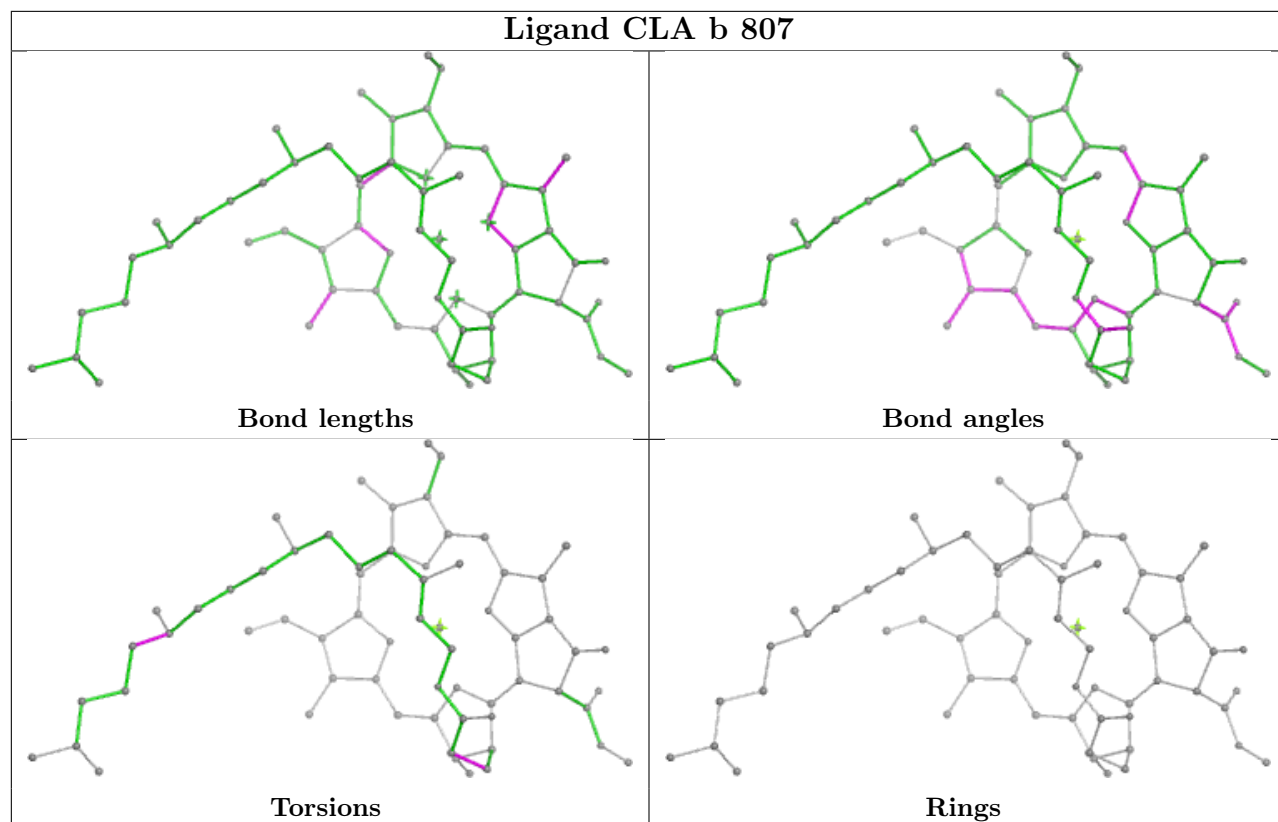


**Ligand F6C a 856****Ligand CLA b 809**

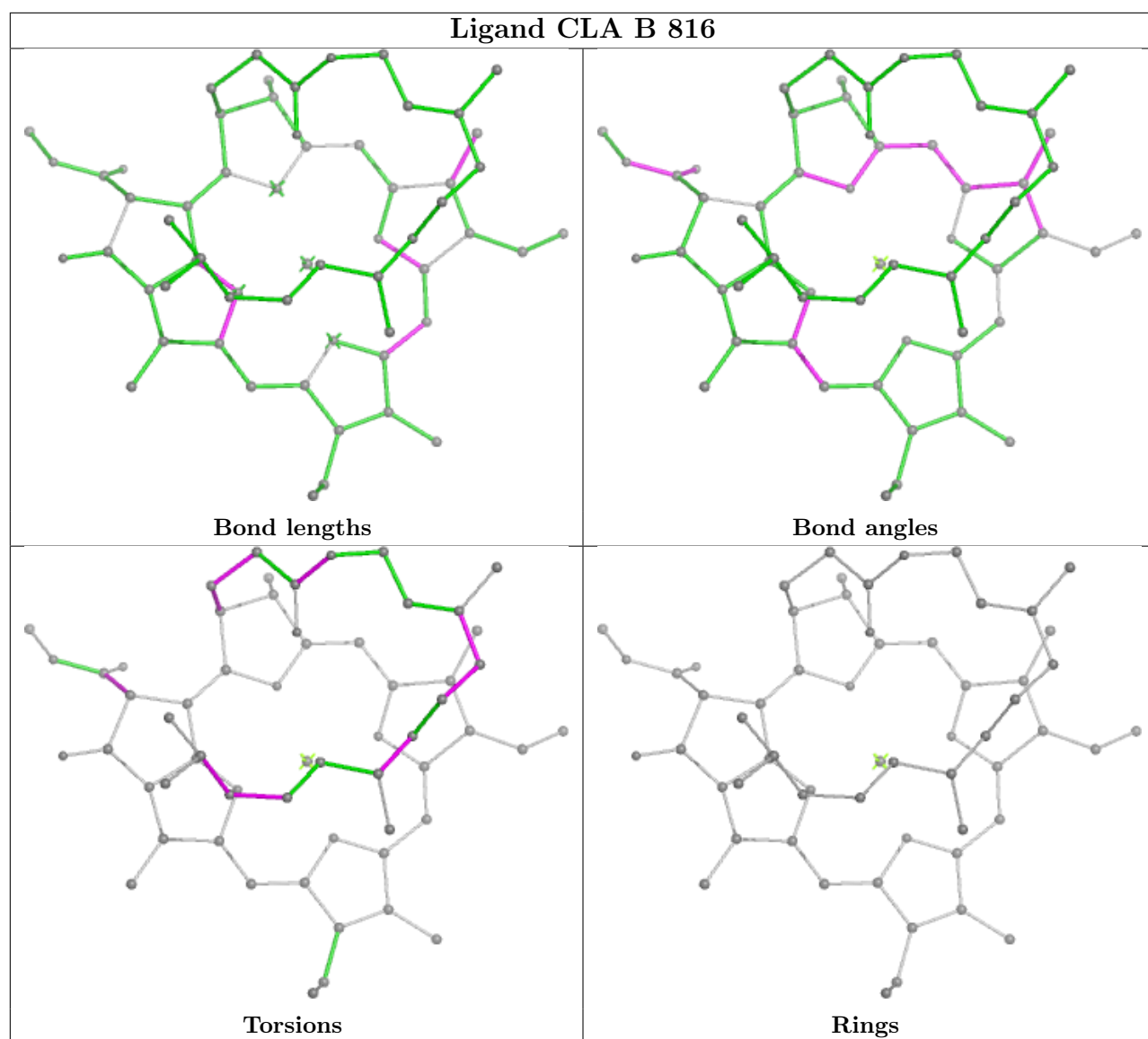




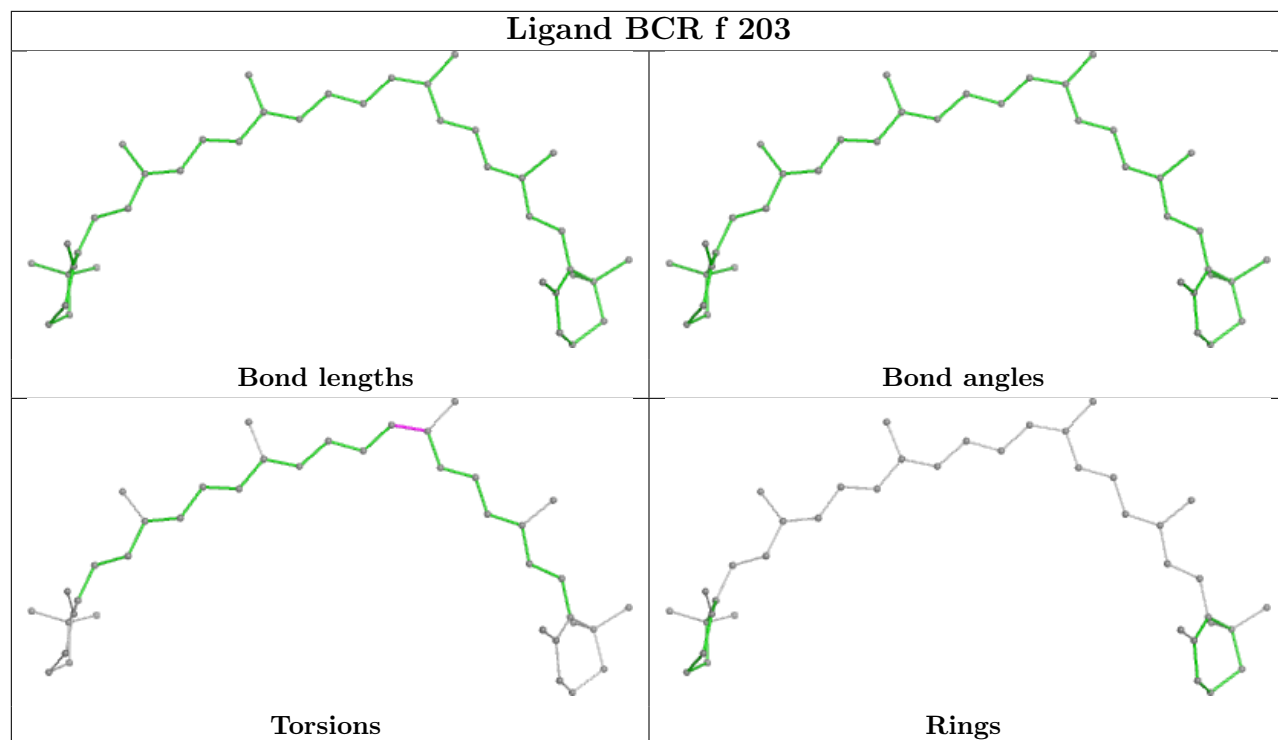
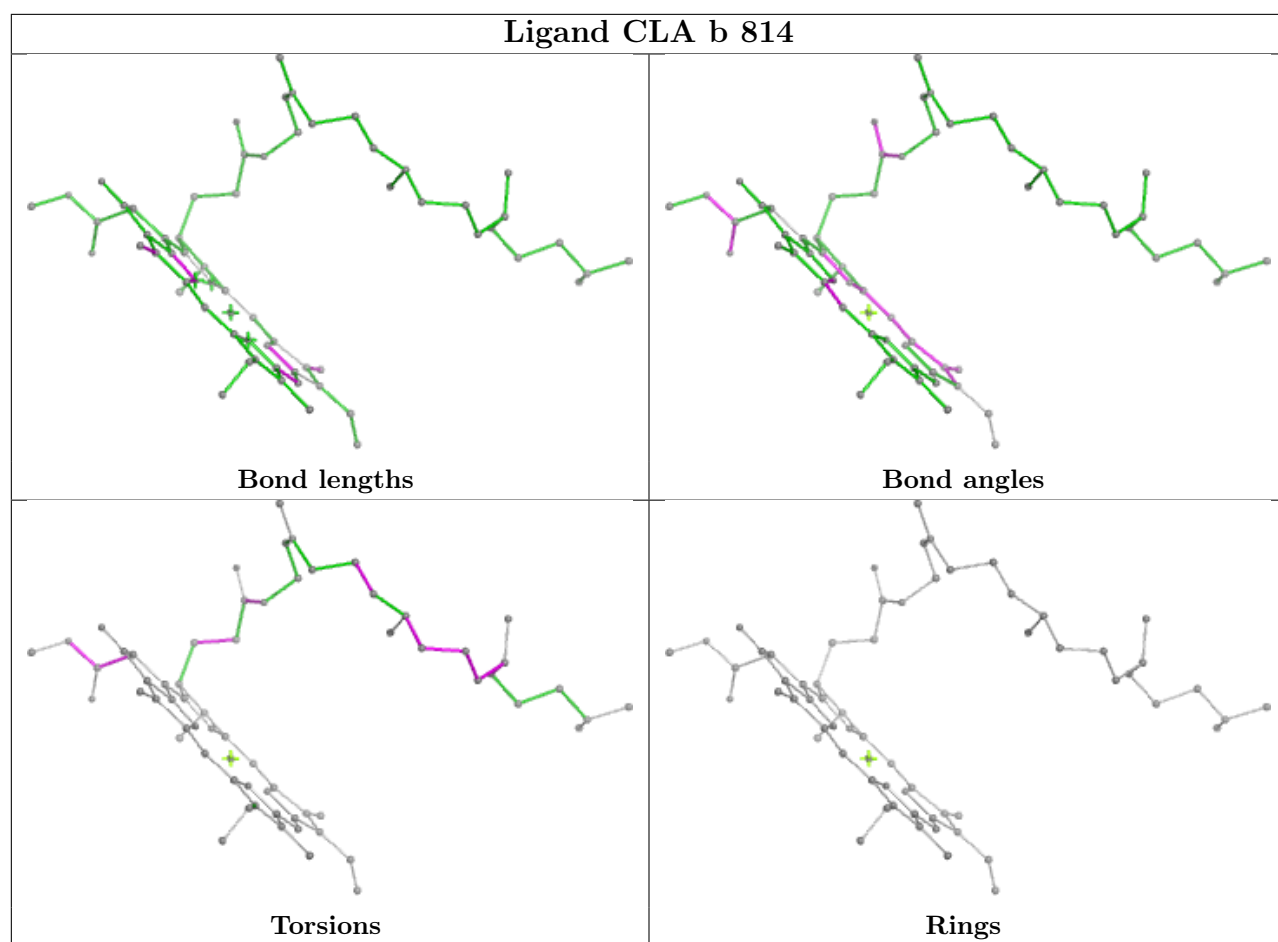






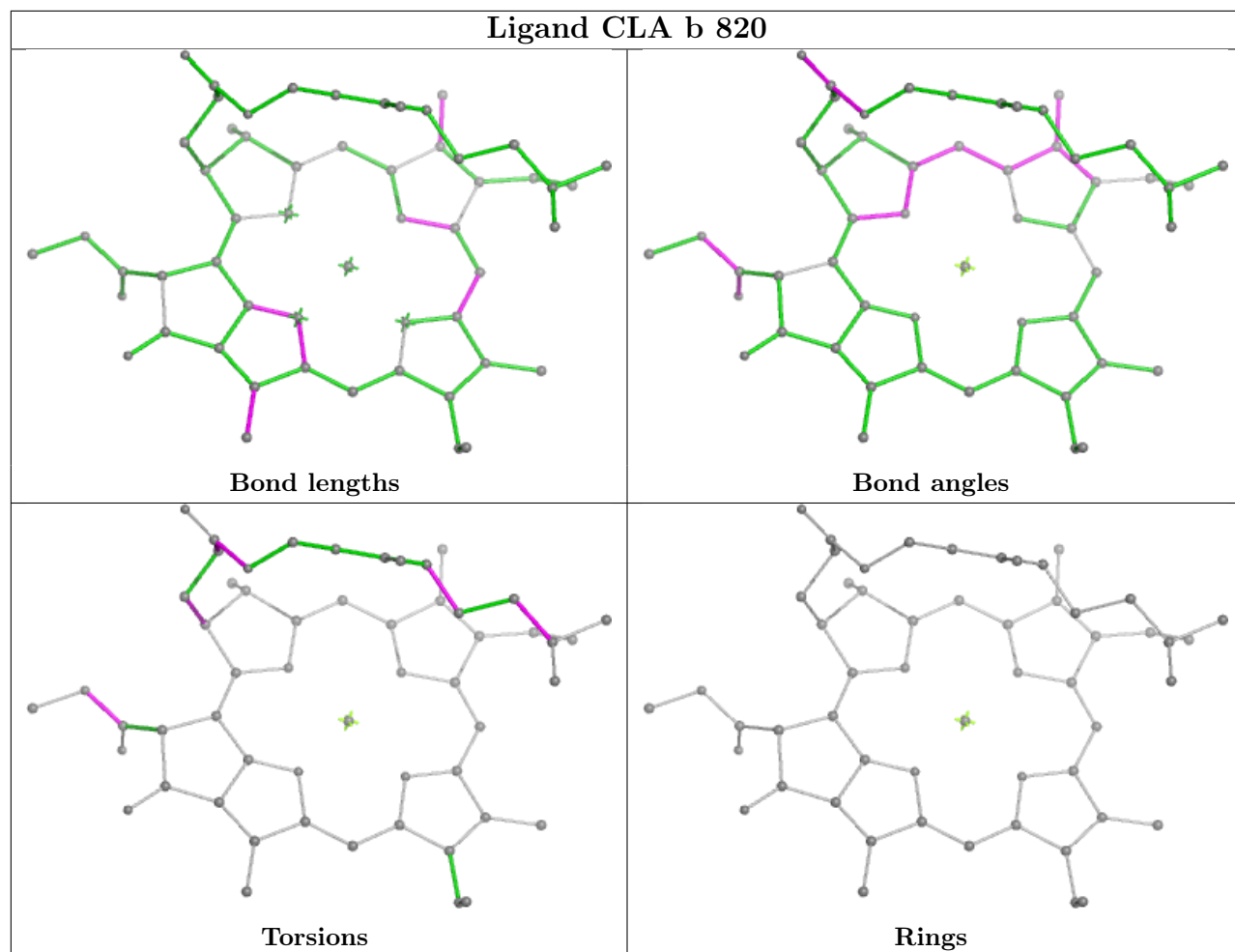






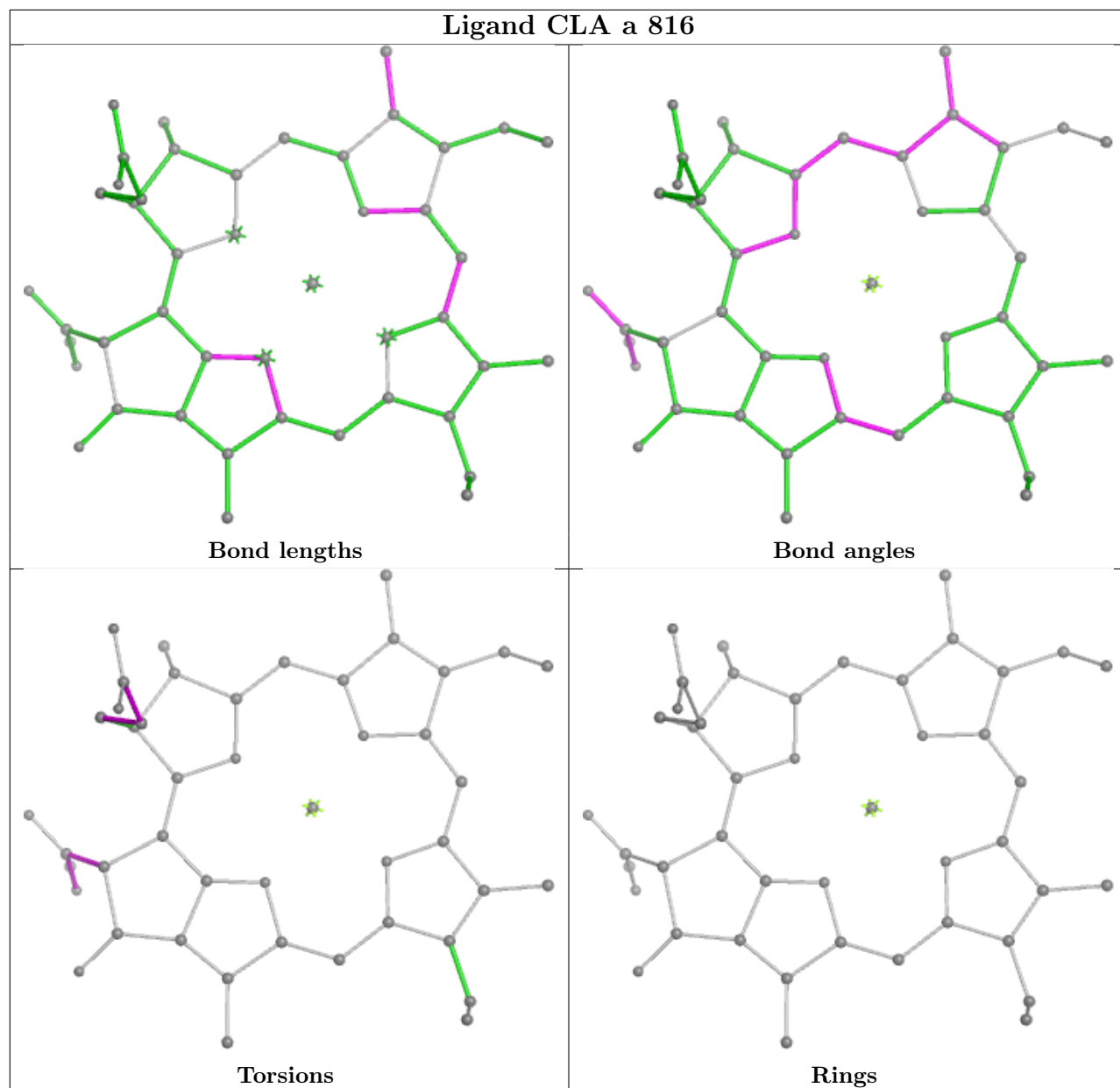


## Ligand CLA b 820

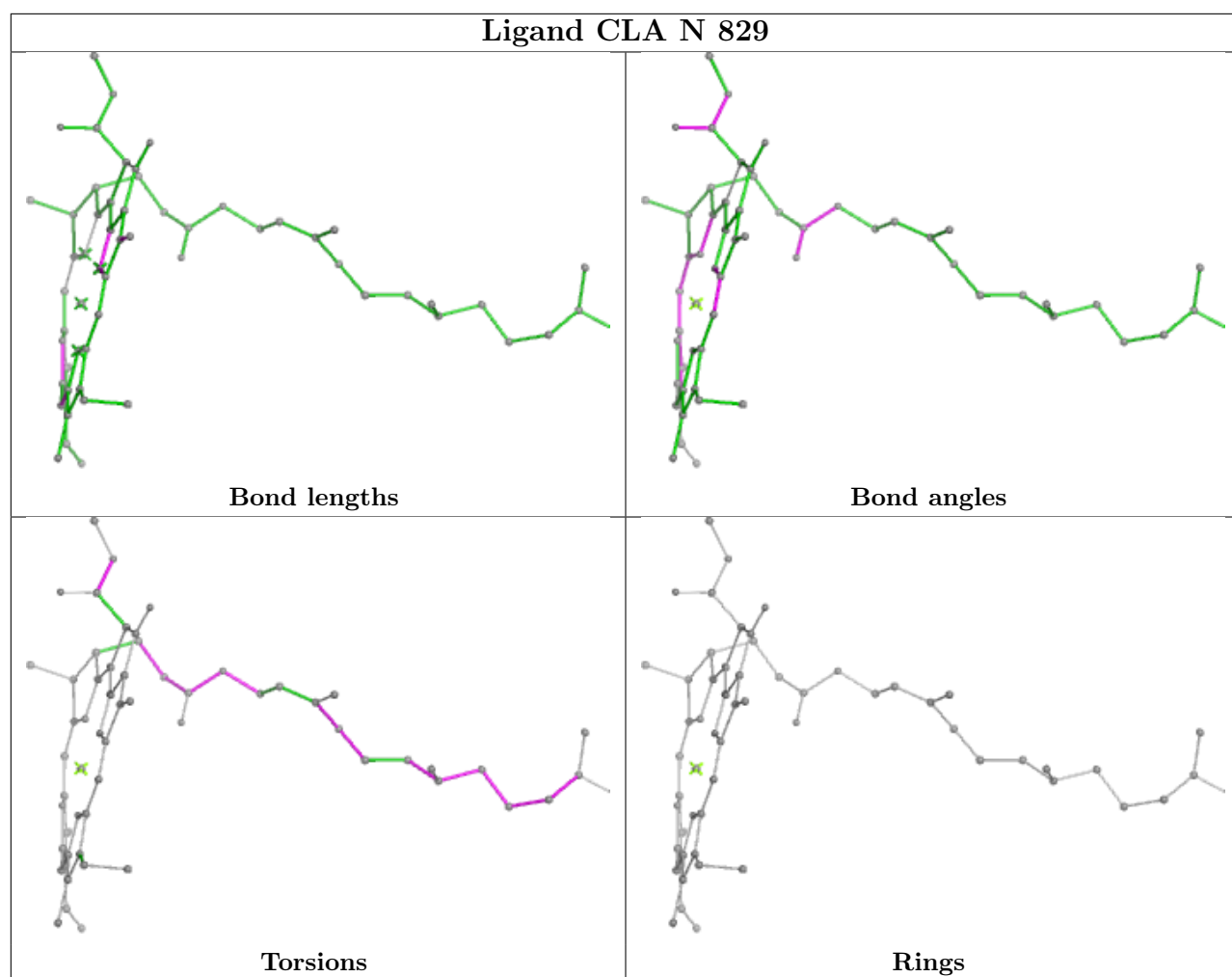




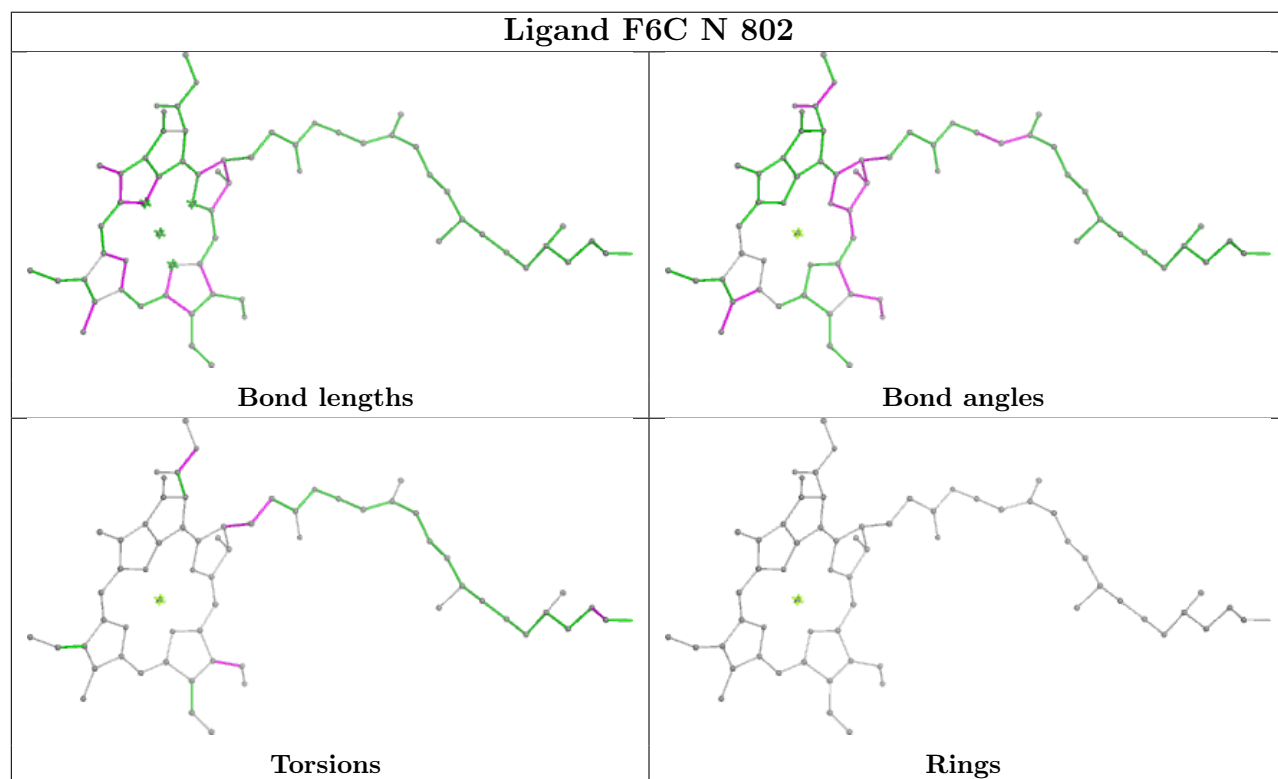
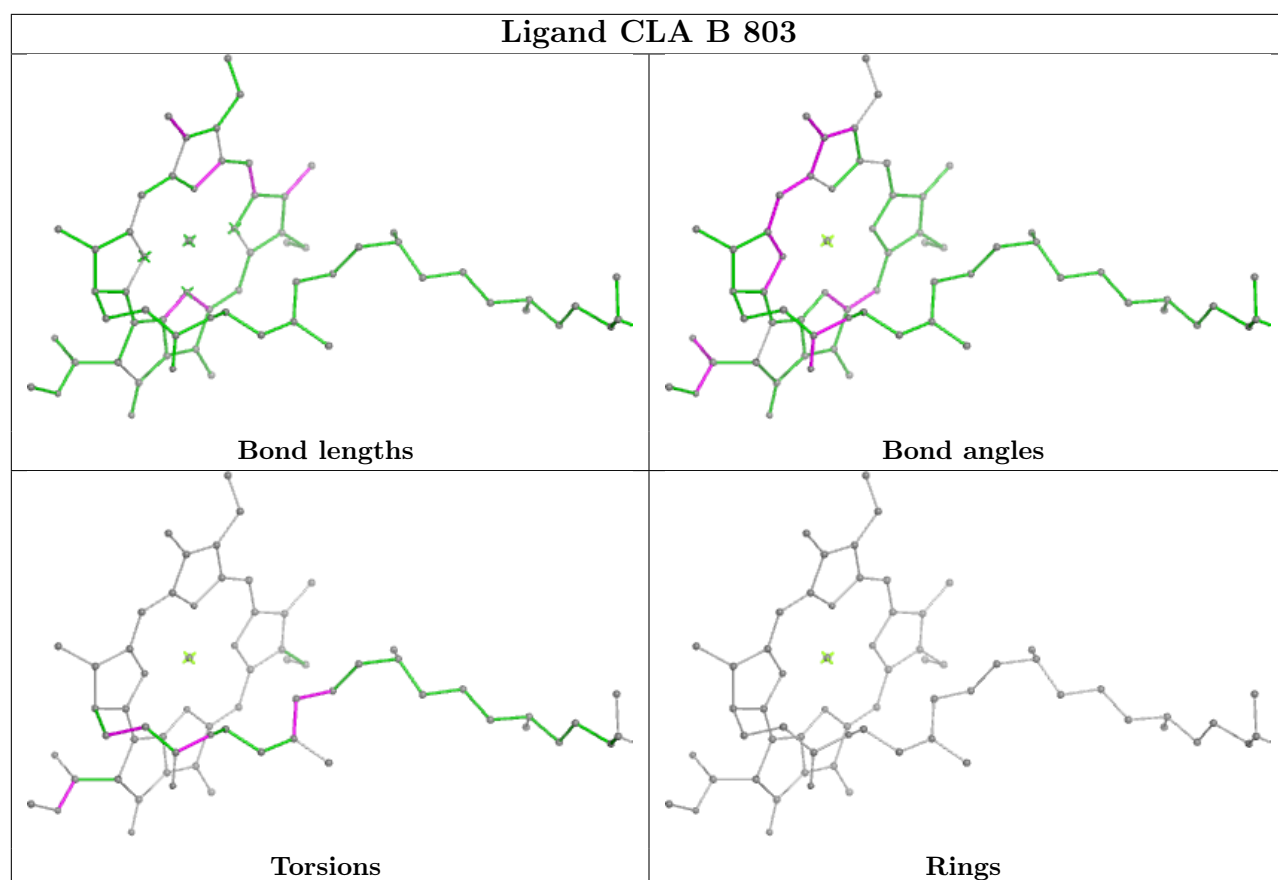
## Ligand CLA a 816





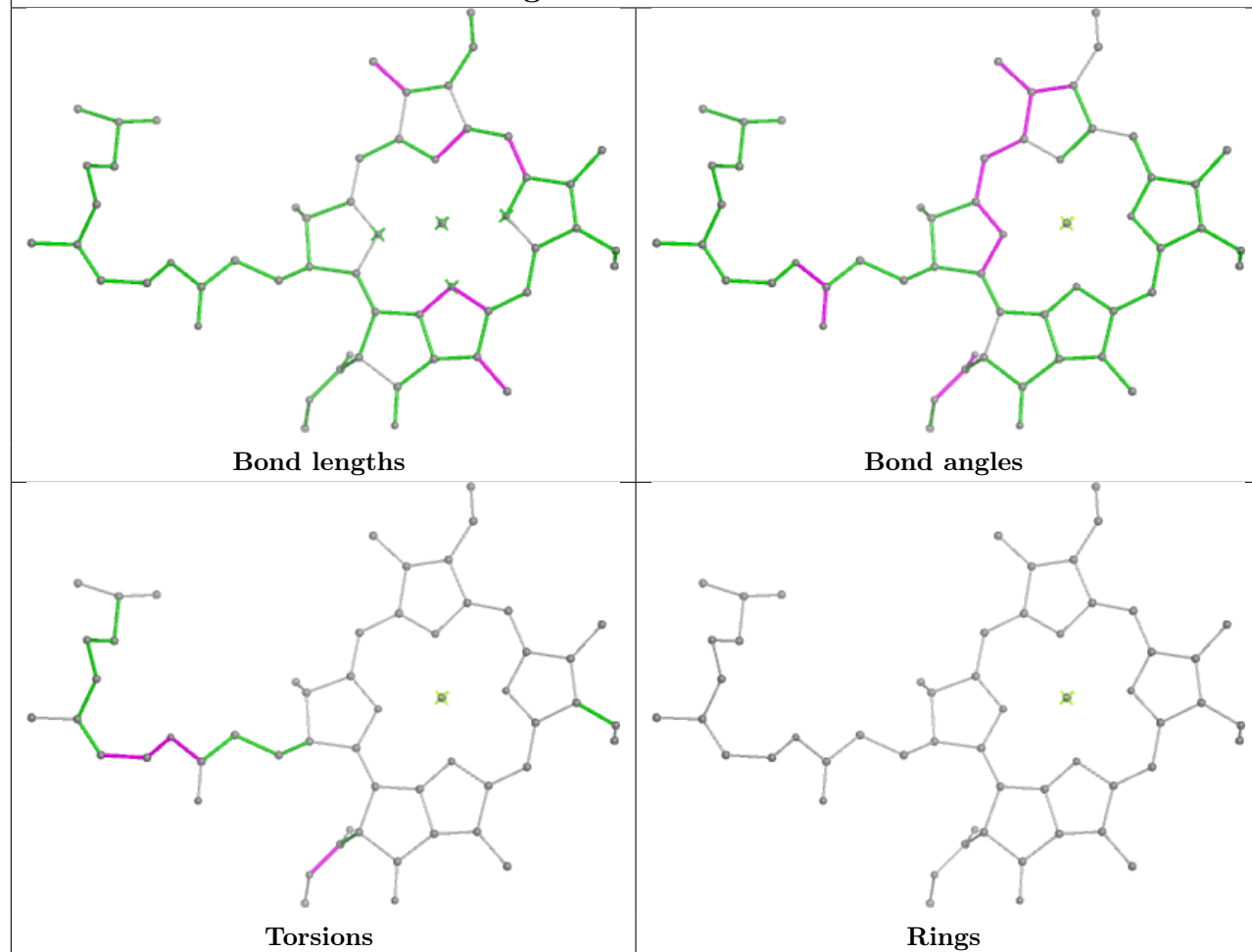




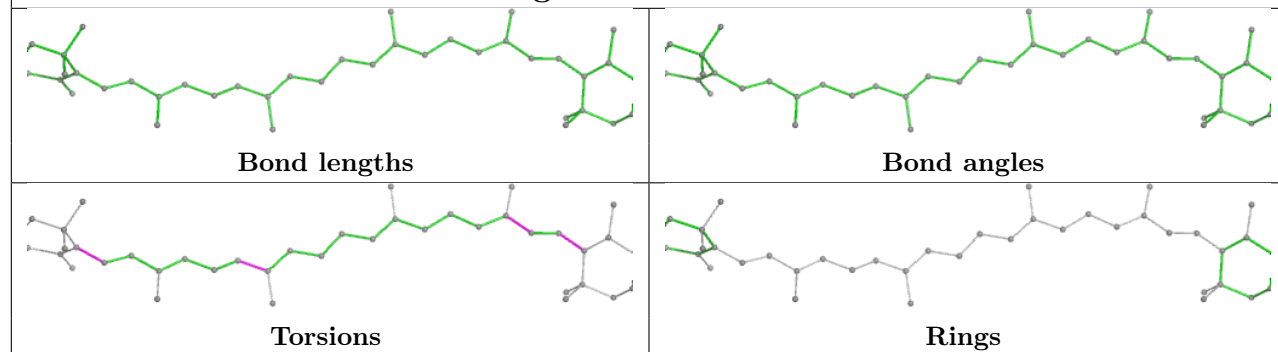




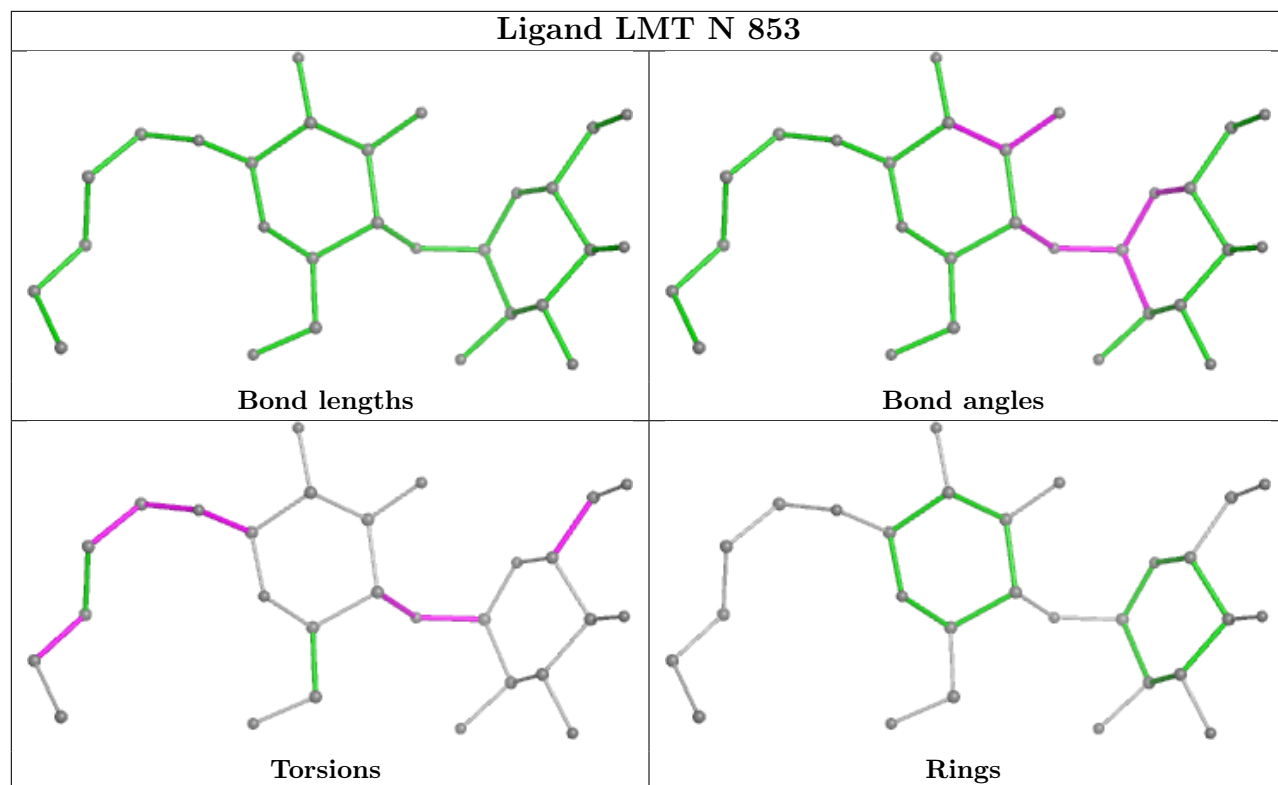
## Ligand CLA Z 103



## Ligand BCR h 101

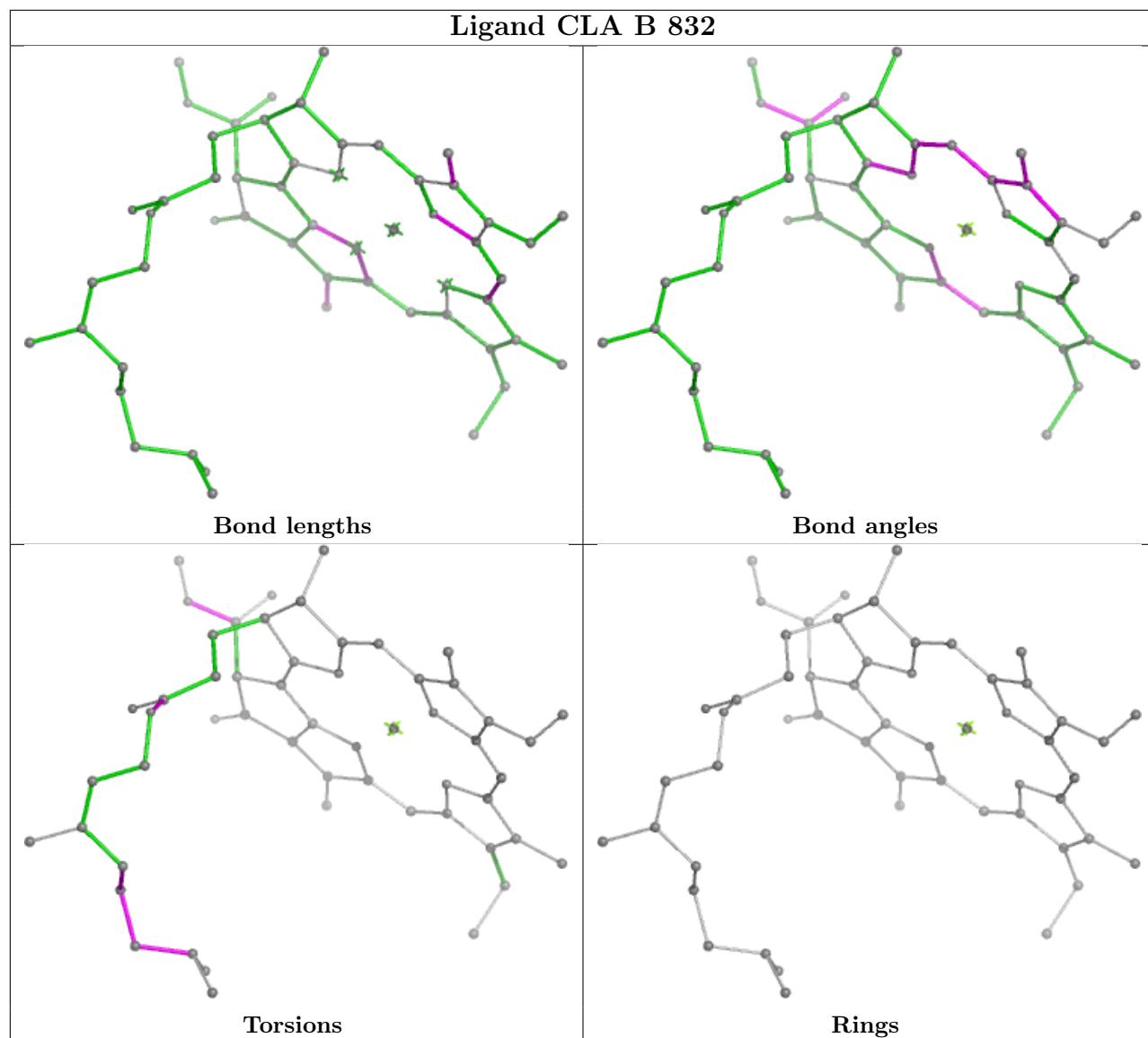






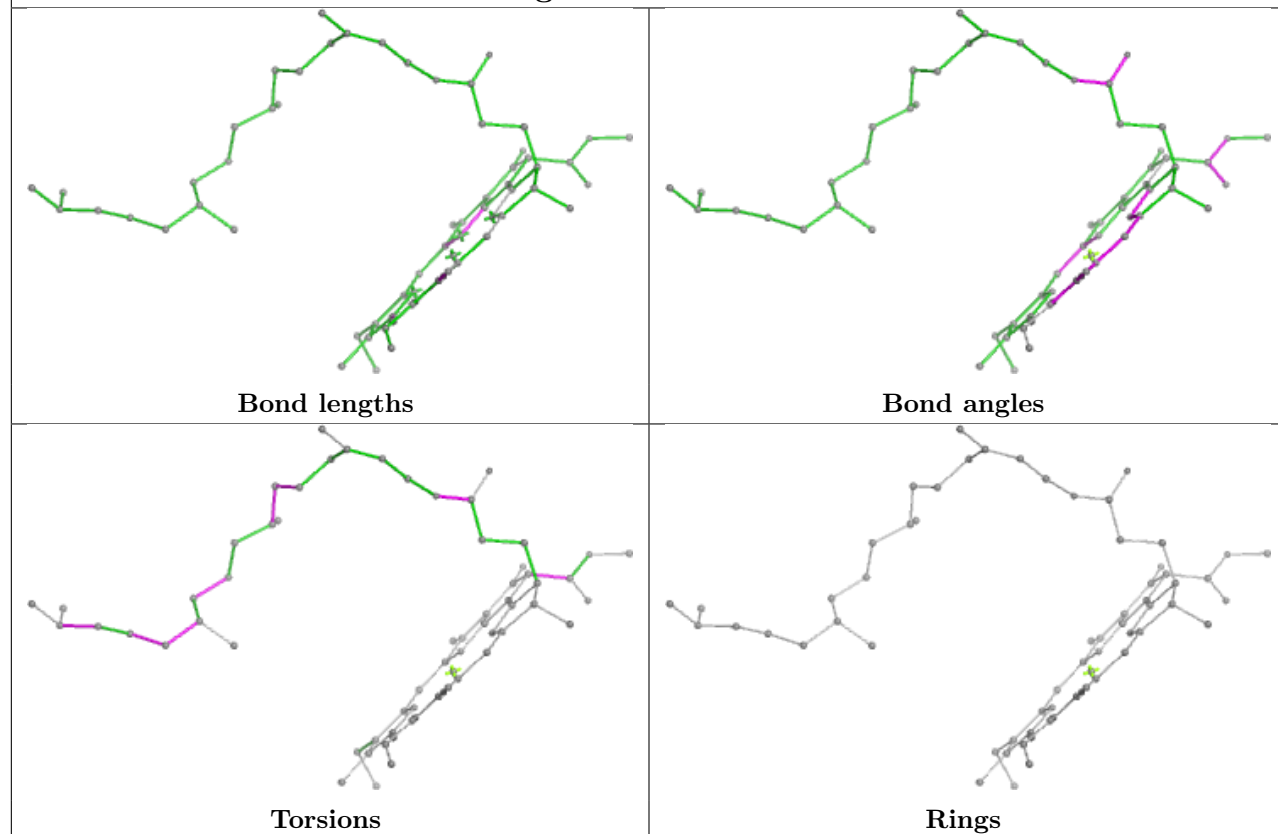


## Ligand CLA B 832

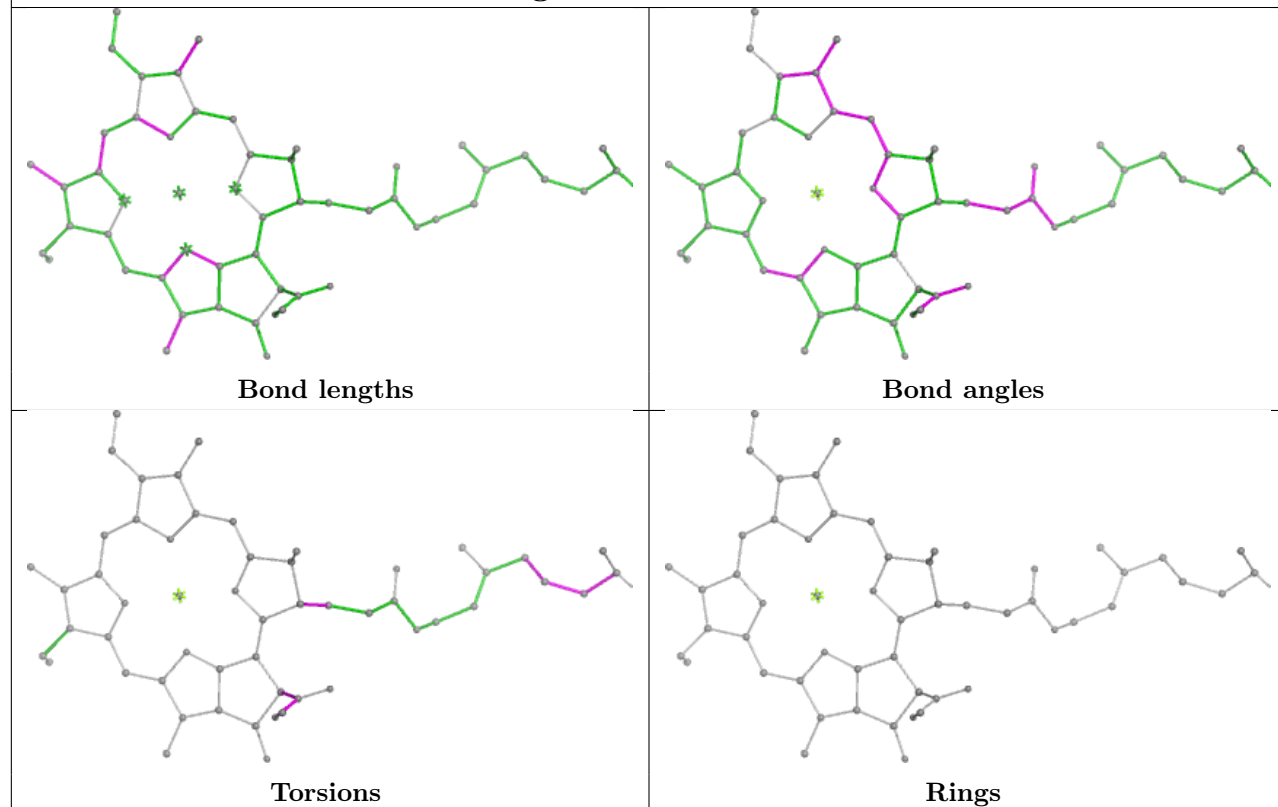




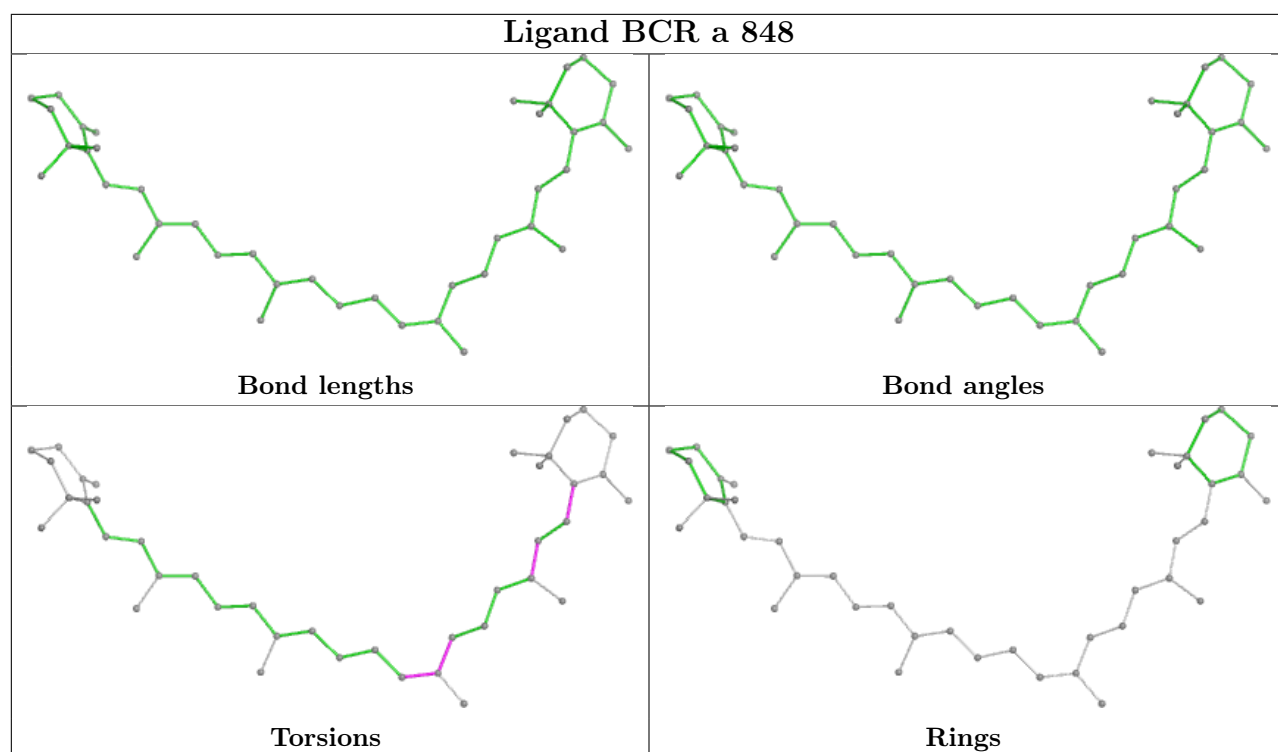
## Ligand CLA b 811



## Ligand CLA O 823

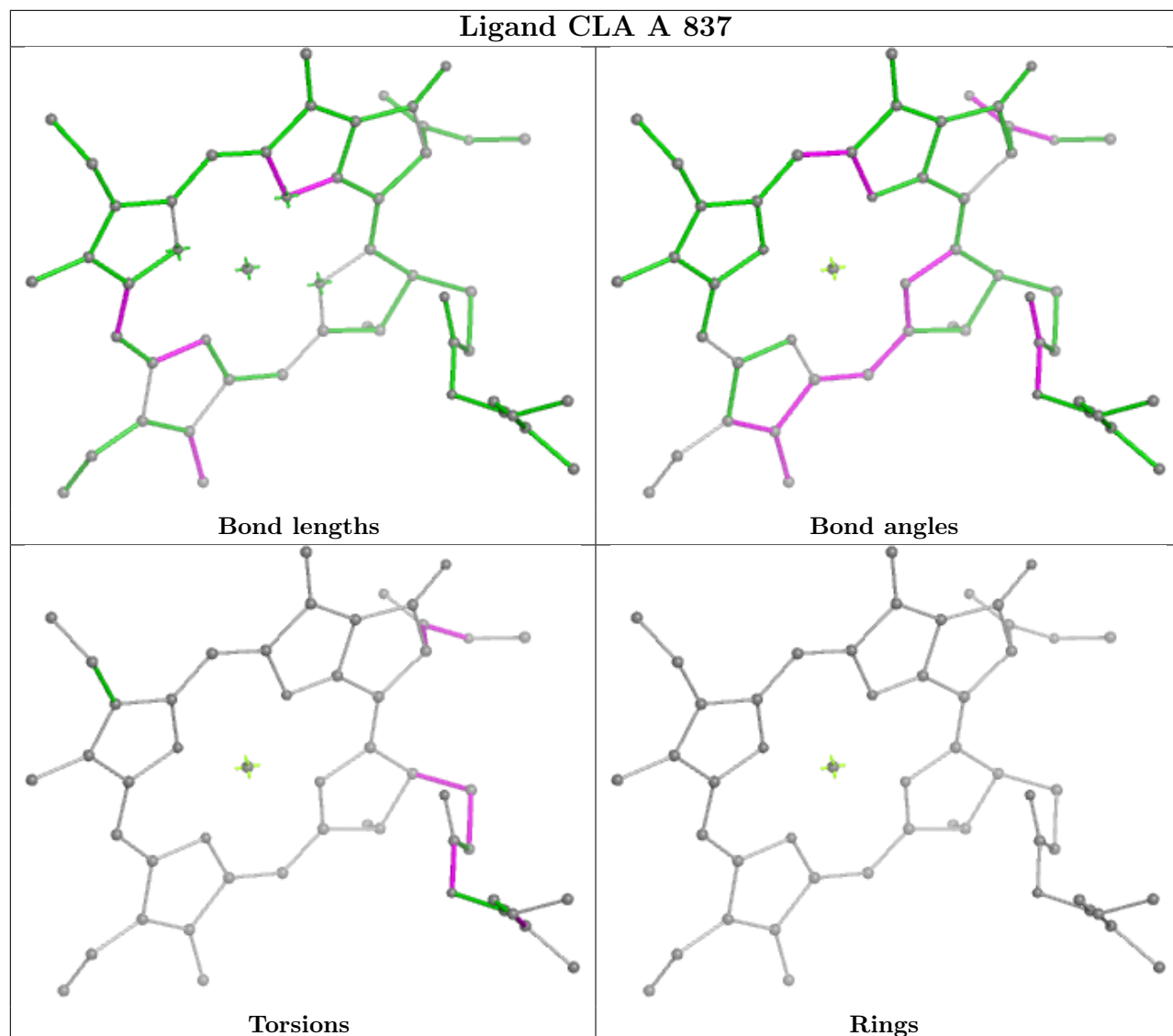




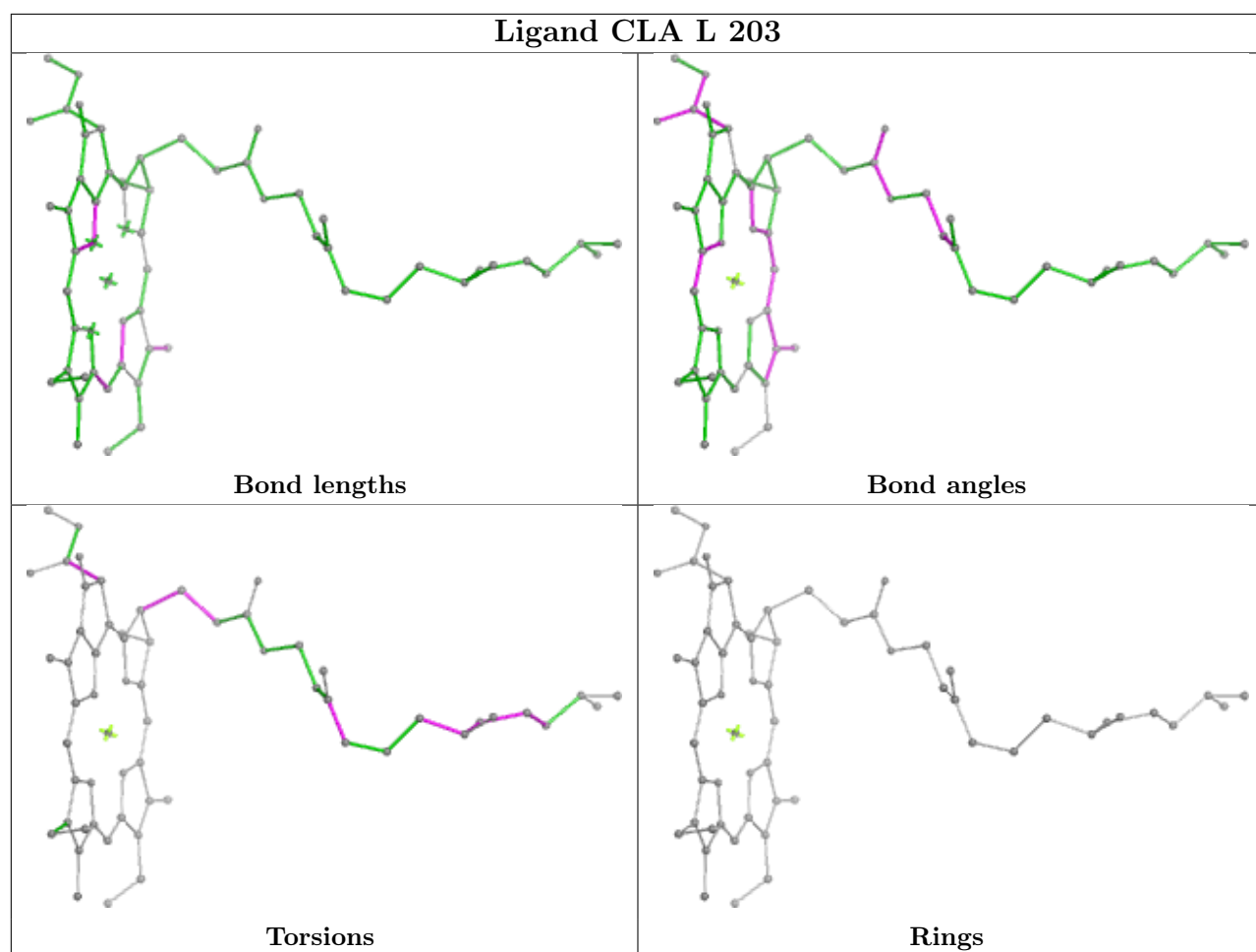




## Ligand CLA A 837

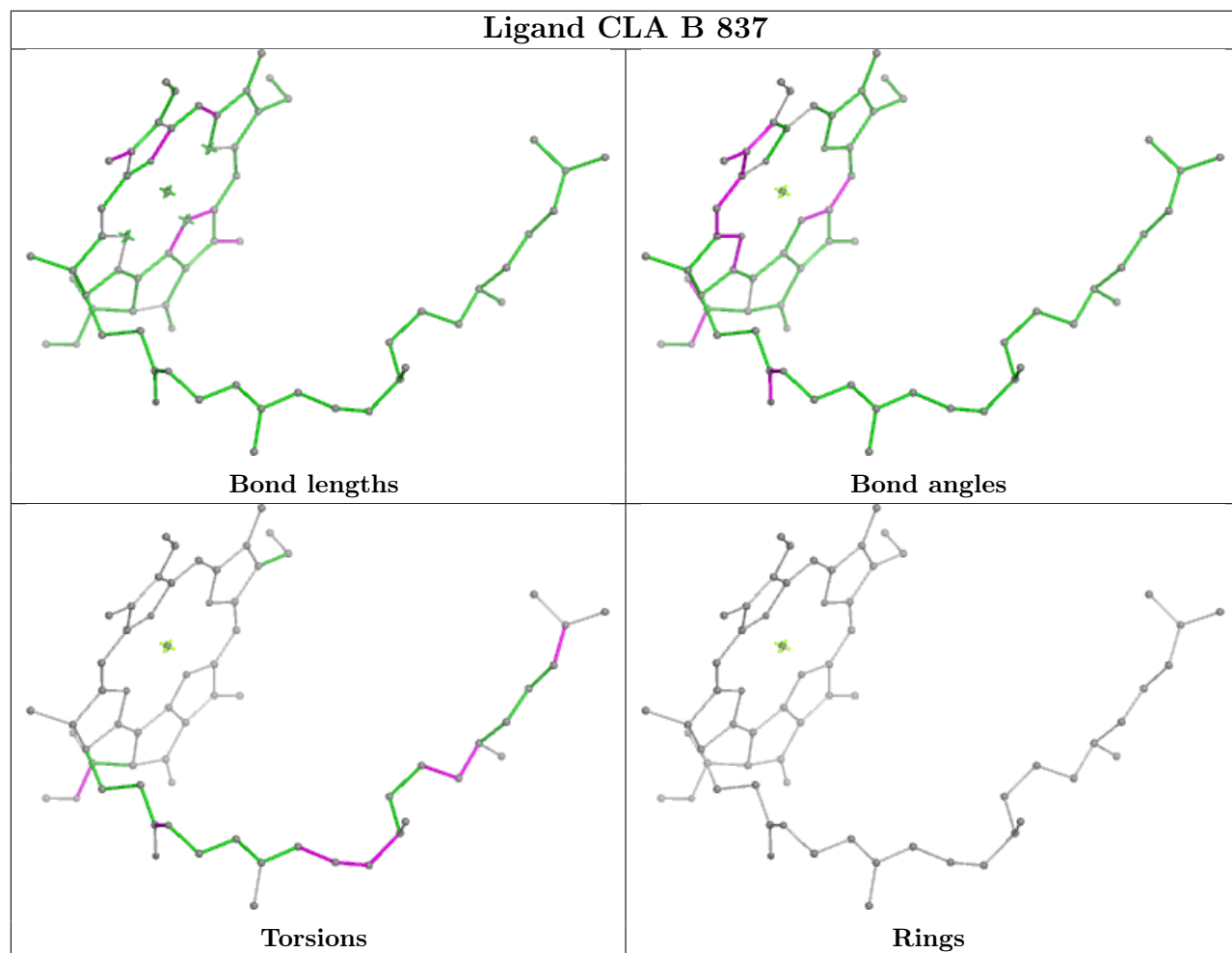




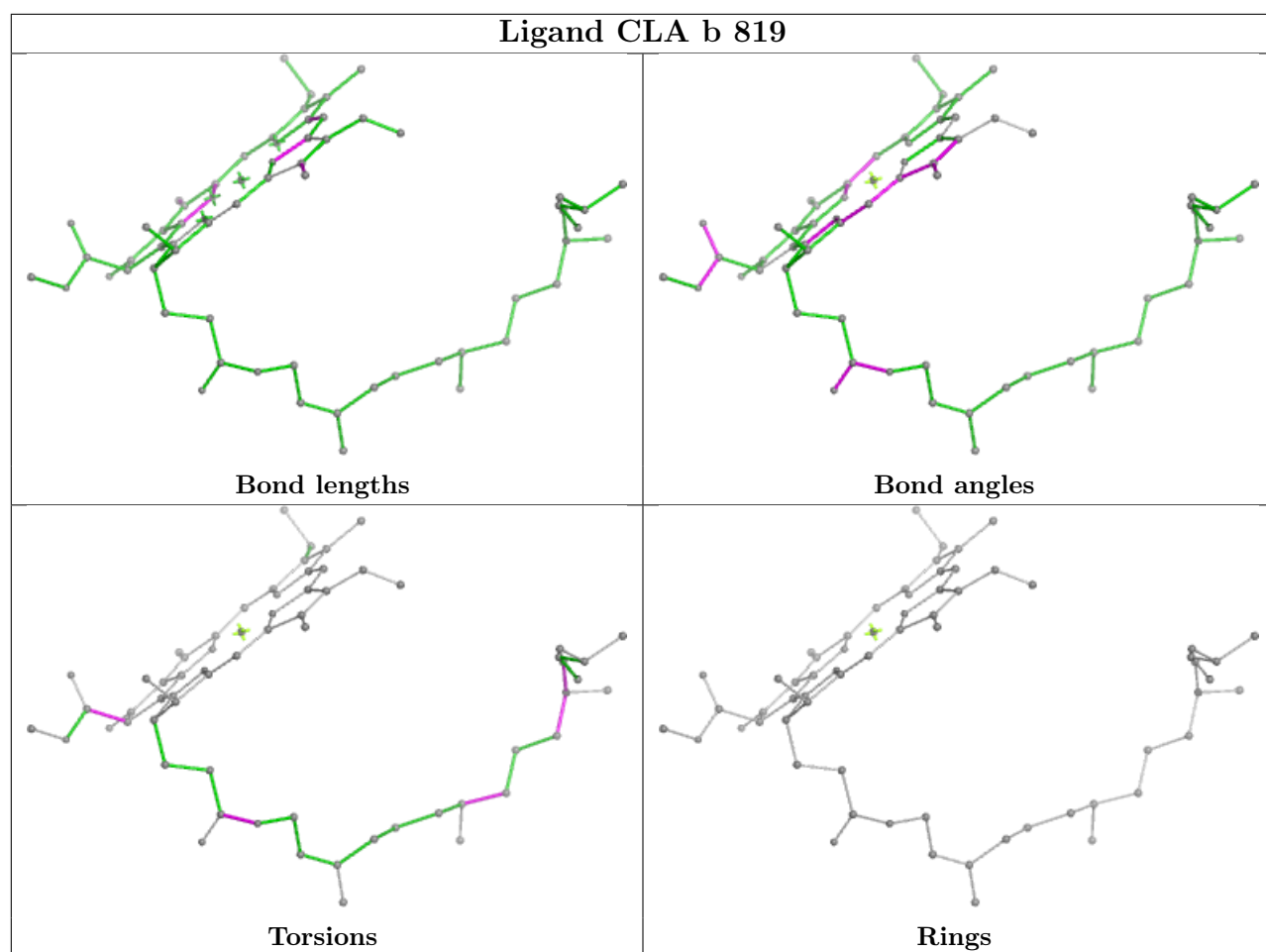




## Ligand CLA B 837

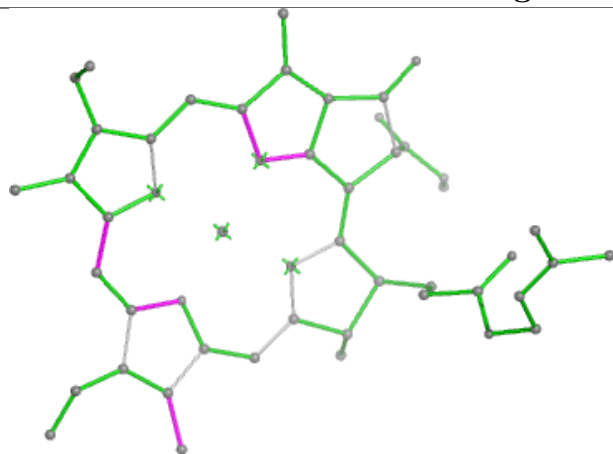




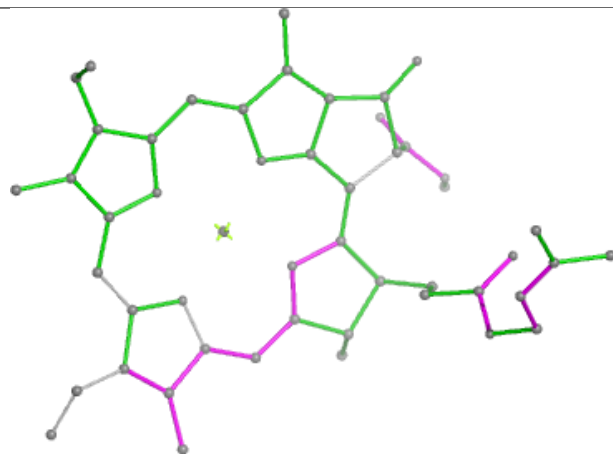




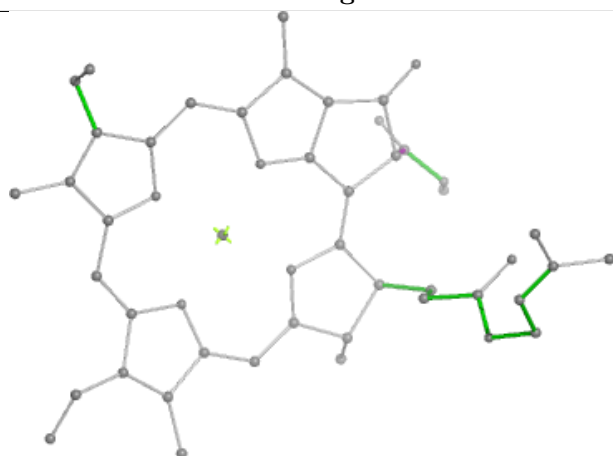
## Ligand CLA A 840



Bond lengths



Bond angles



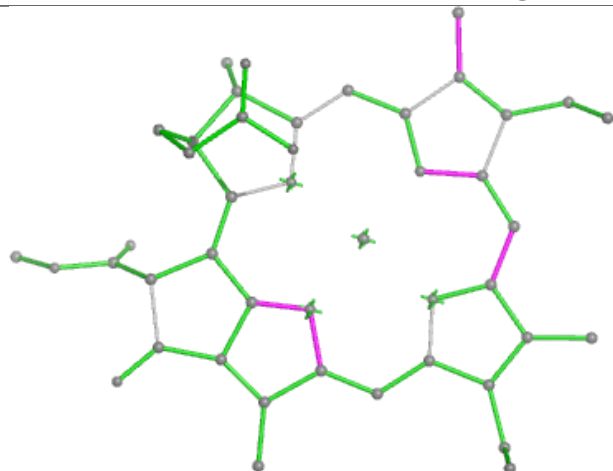
Torsions



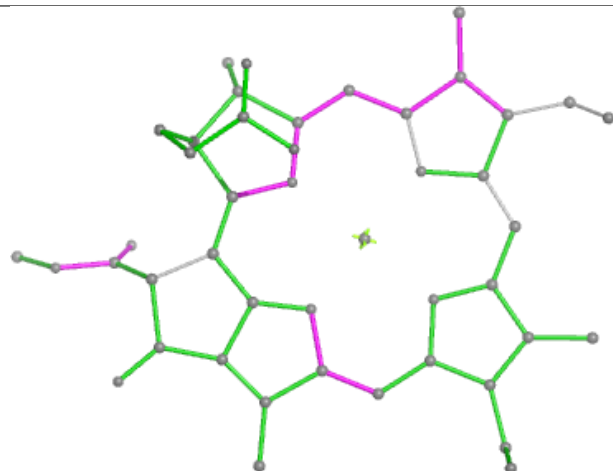
Rings



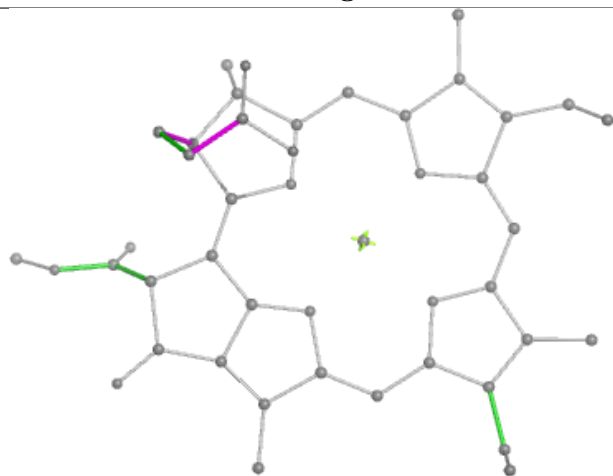
## Ligand CLA O 812



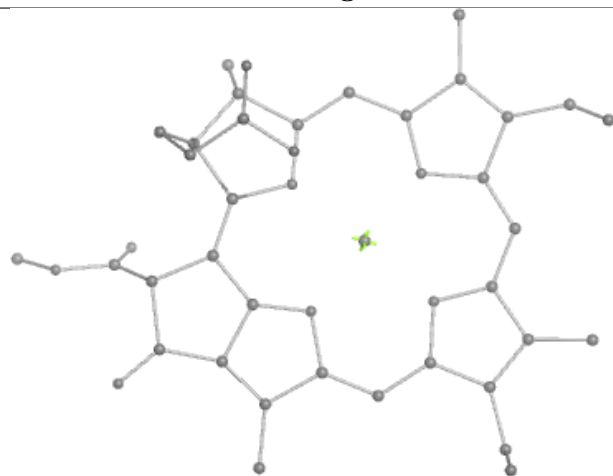
Bond lengths



Bond angles

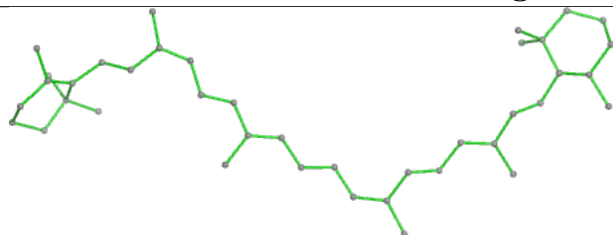


Torsions

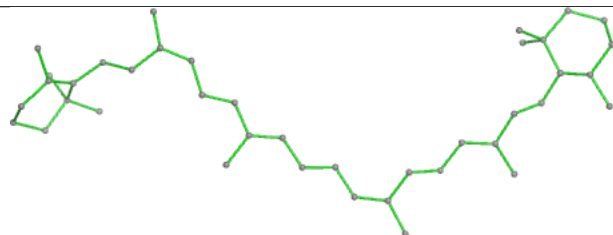


Rings

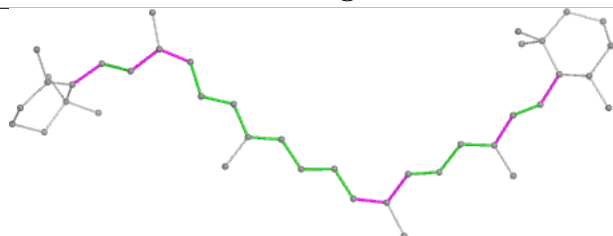
## Ligand BCR N 850



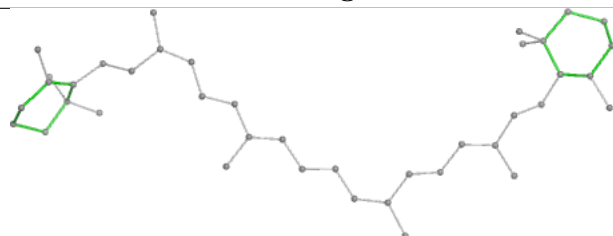
Bond lengths



Bond angles



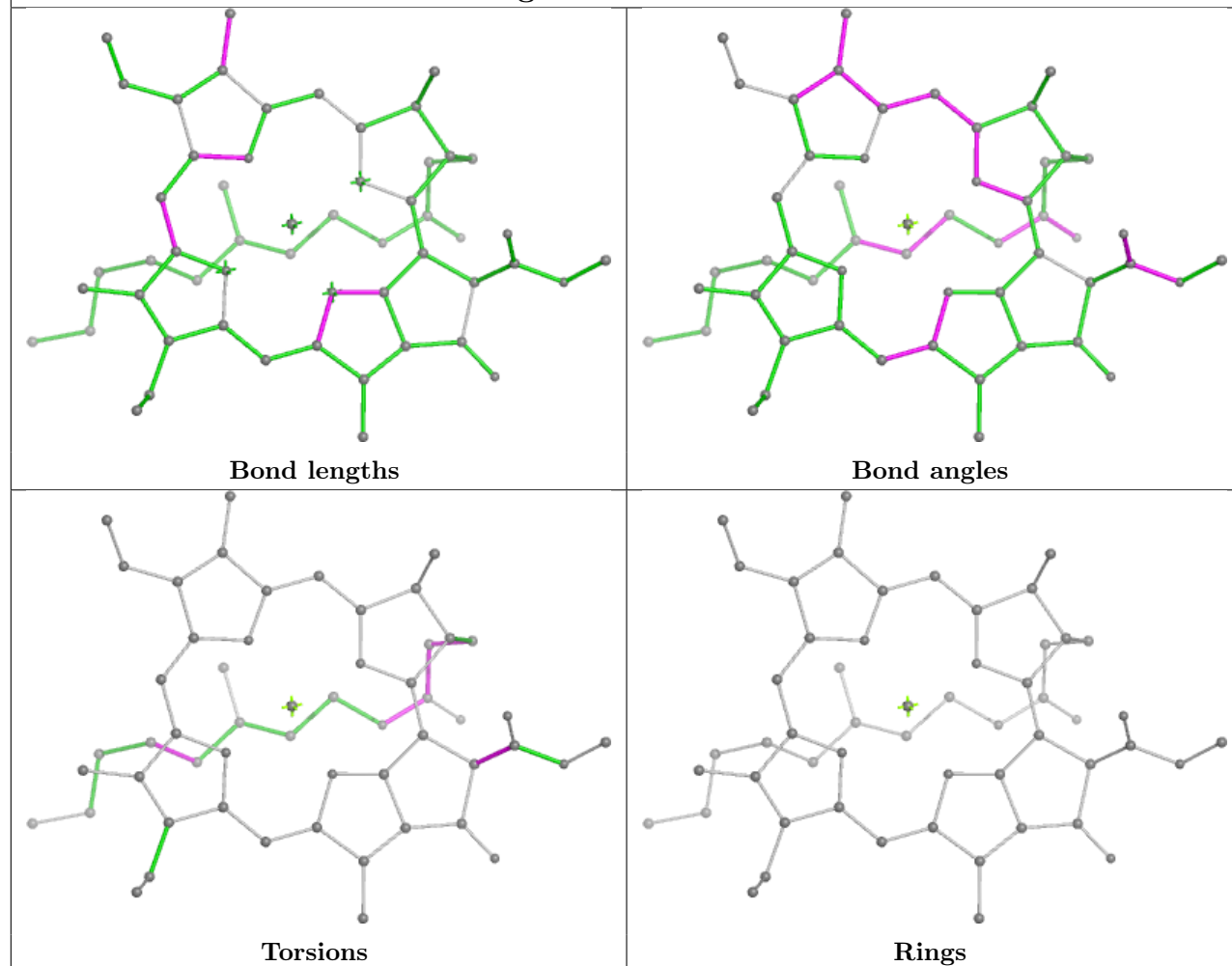
Torsions



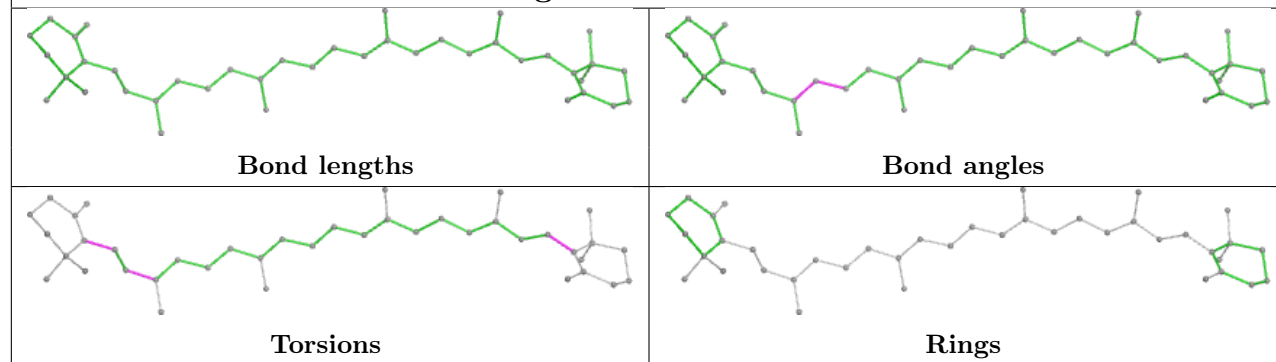
Rings



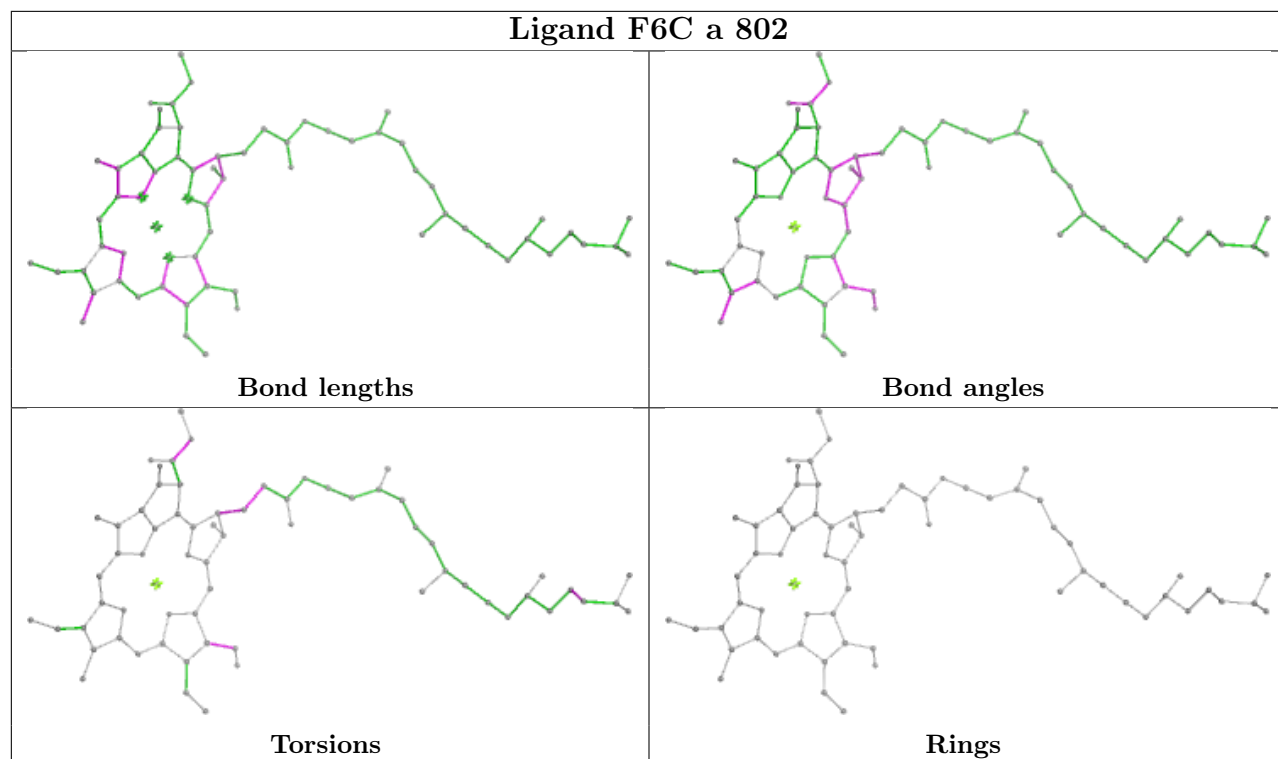
## Ligand CLA a 813



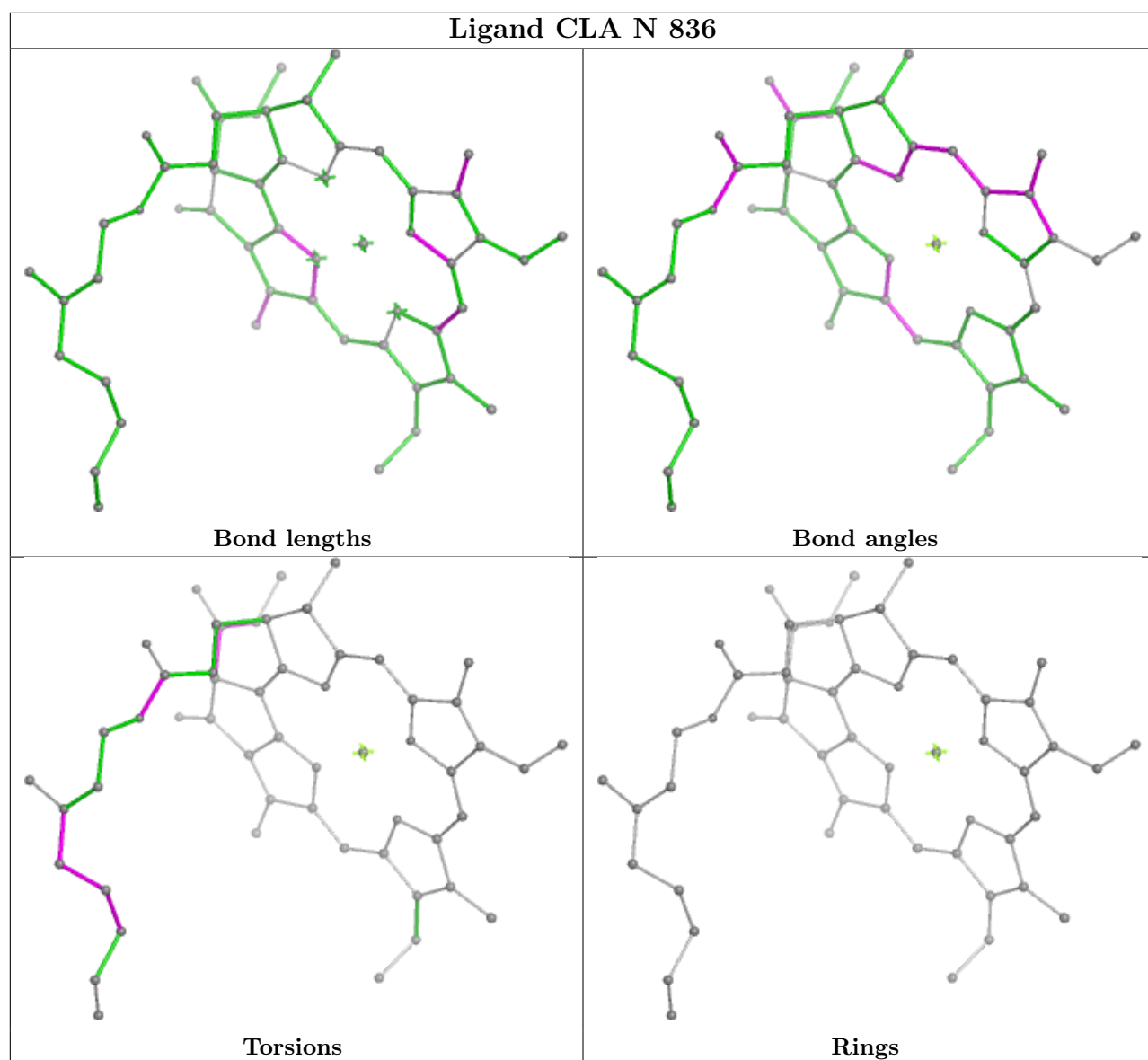
## Ligand BCR a 847



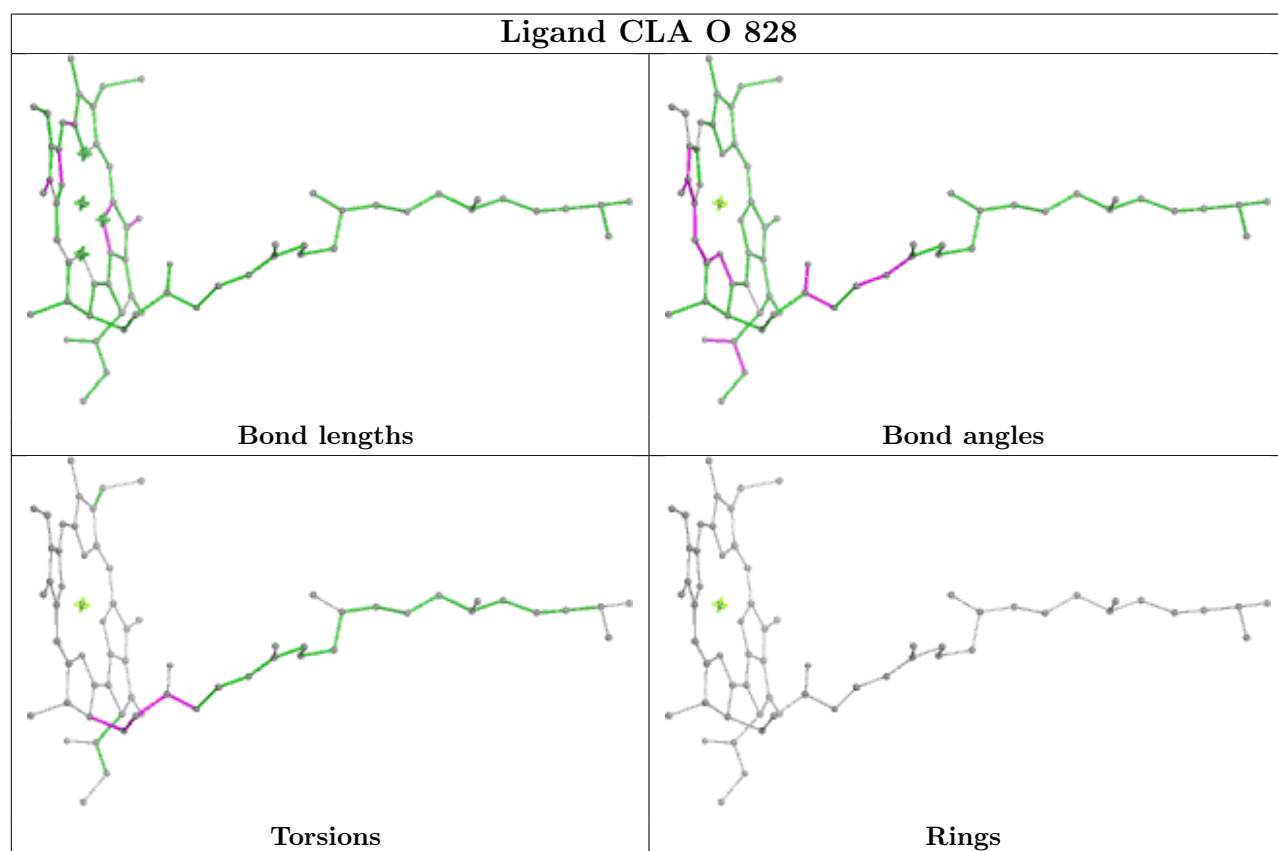
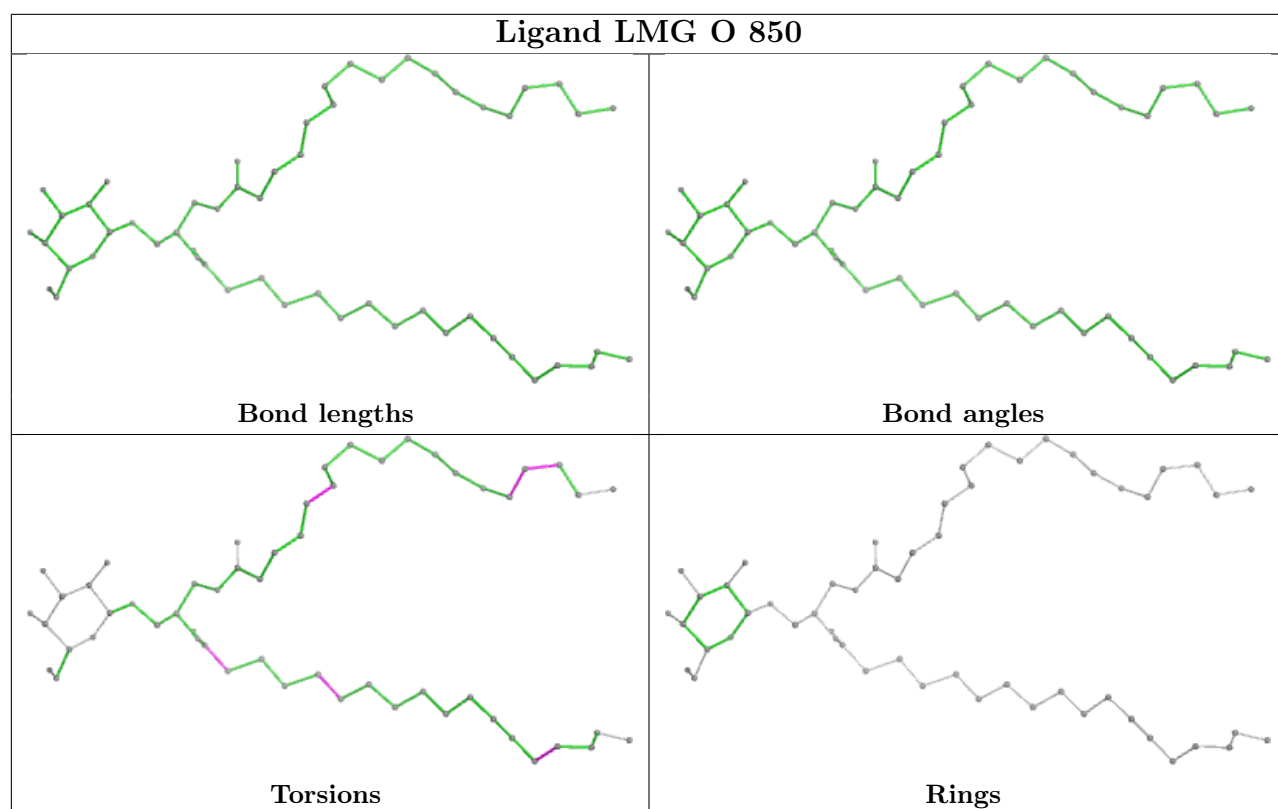




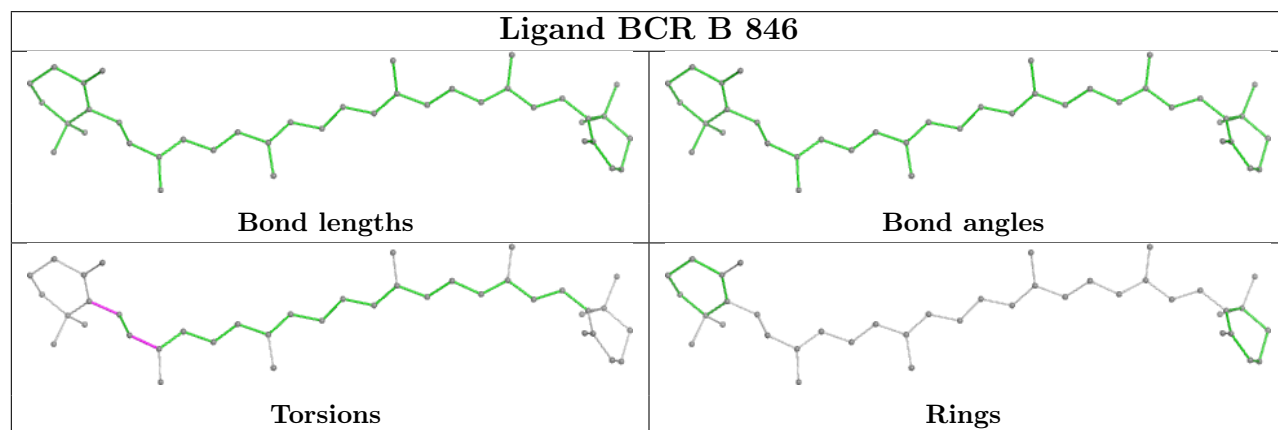
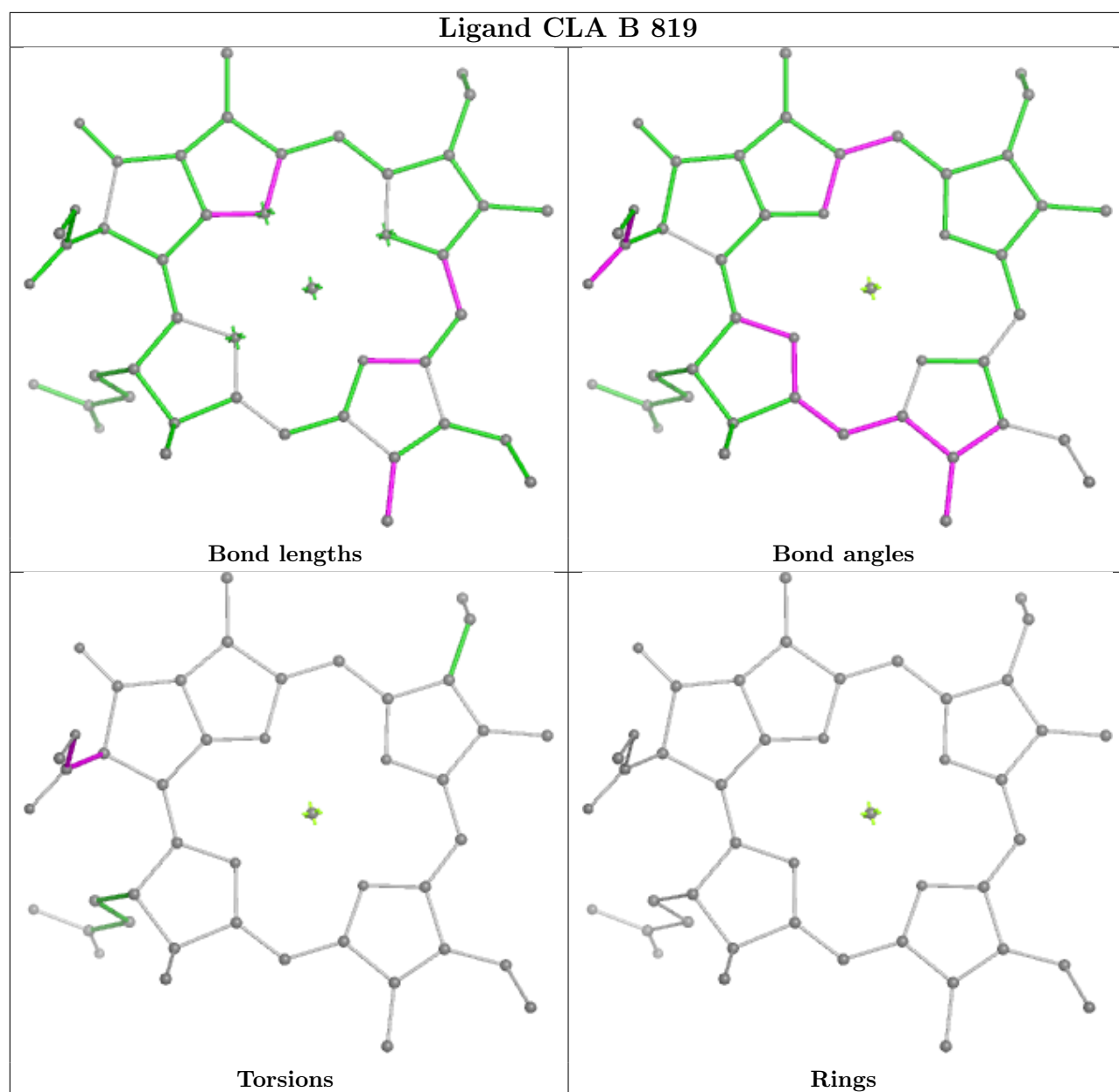




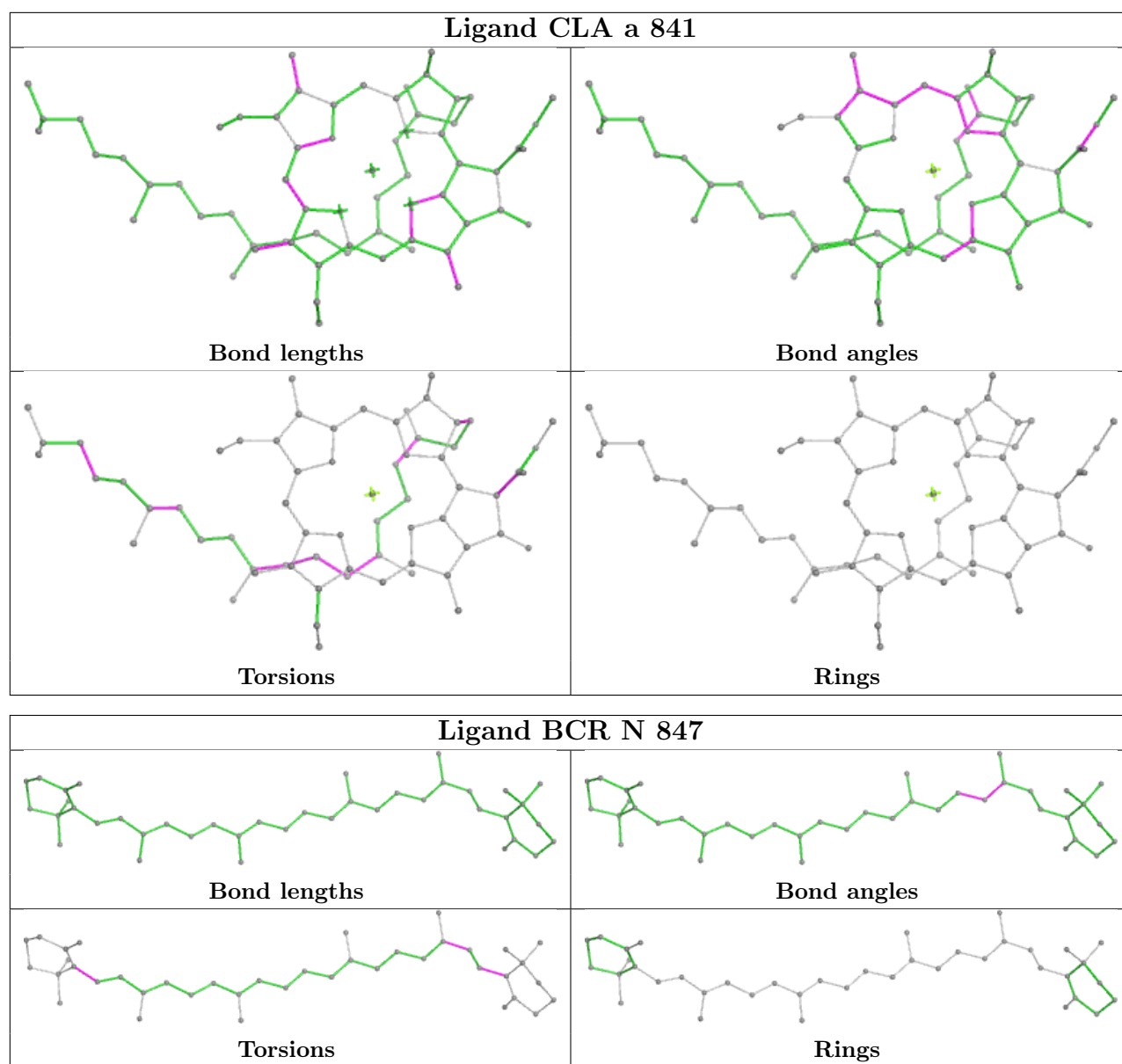






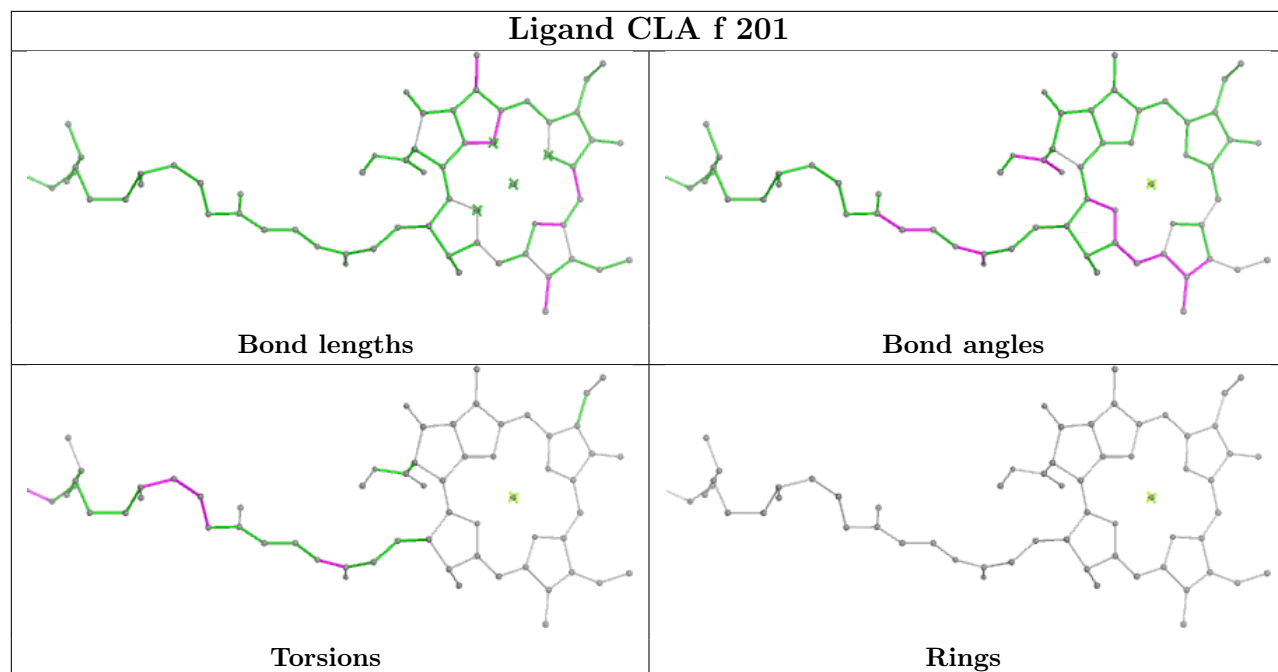




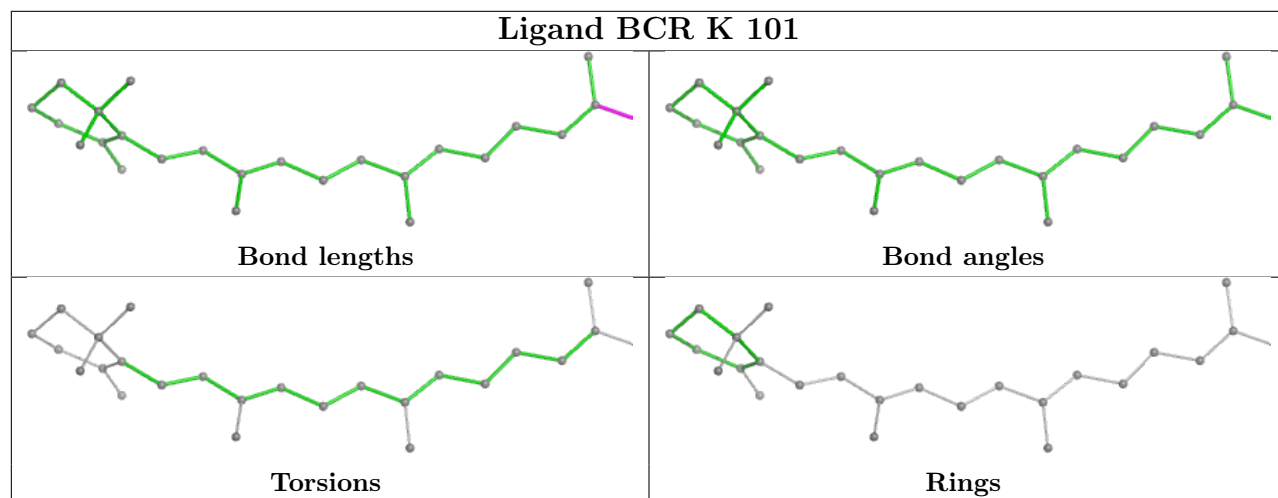




## Ligand CLA f 201

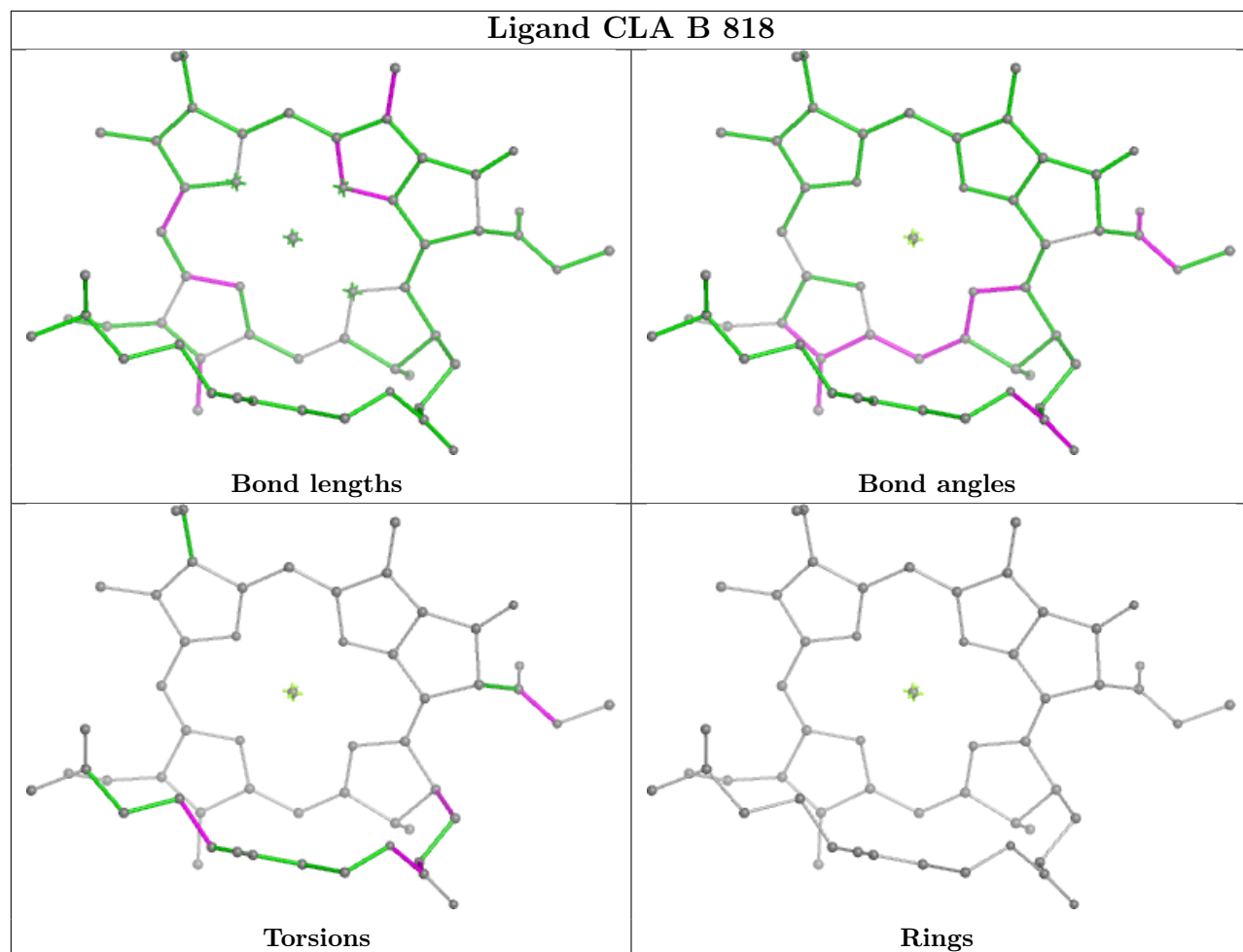


## Ligand BCR K 101

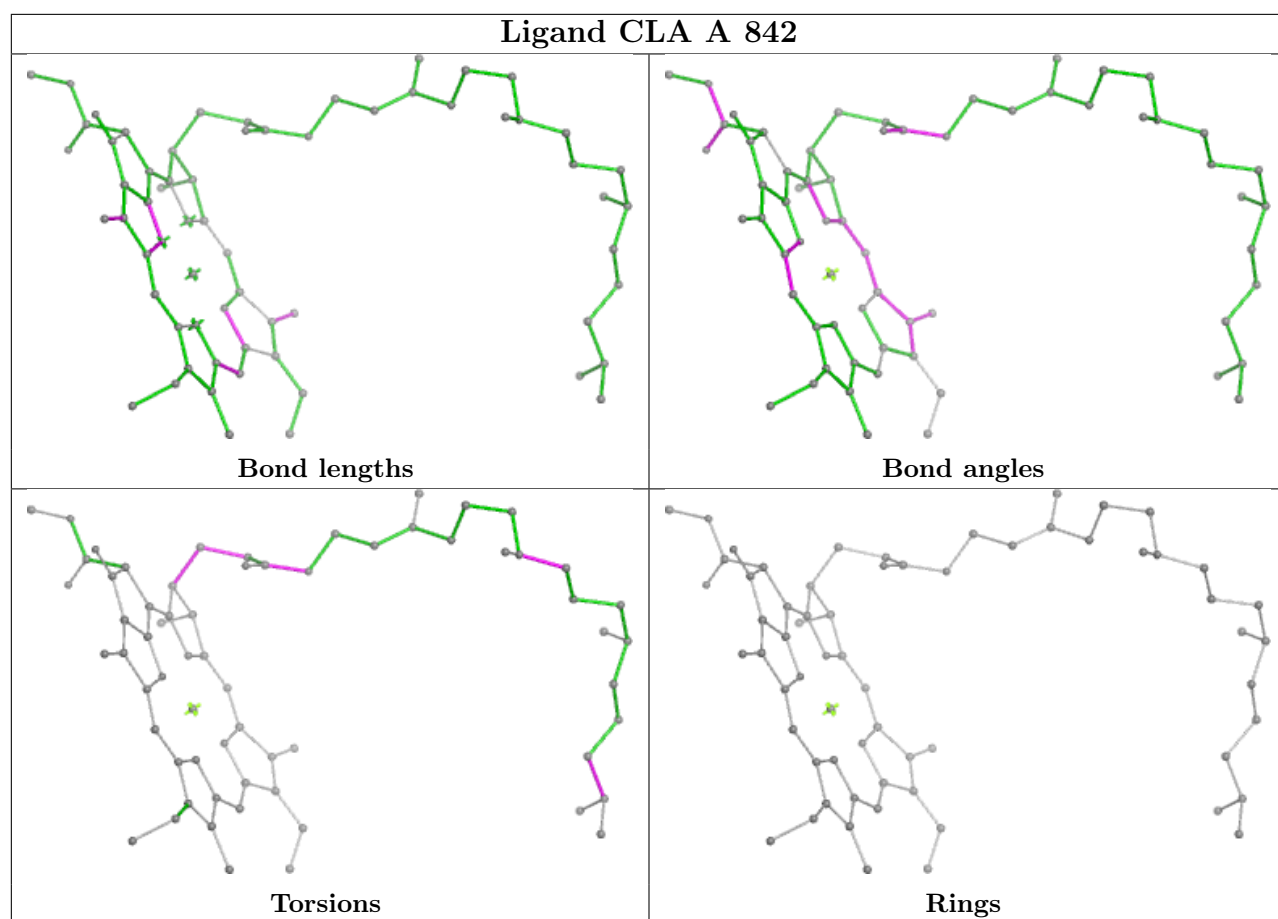




## Ligand CLA B 818

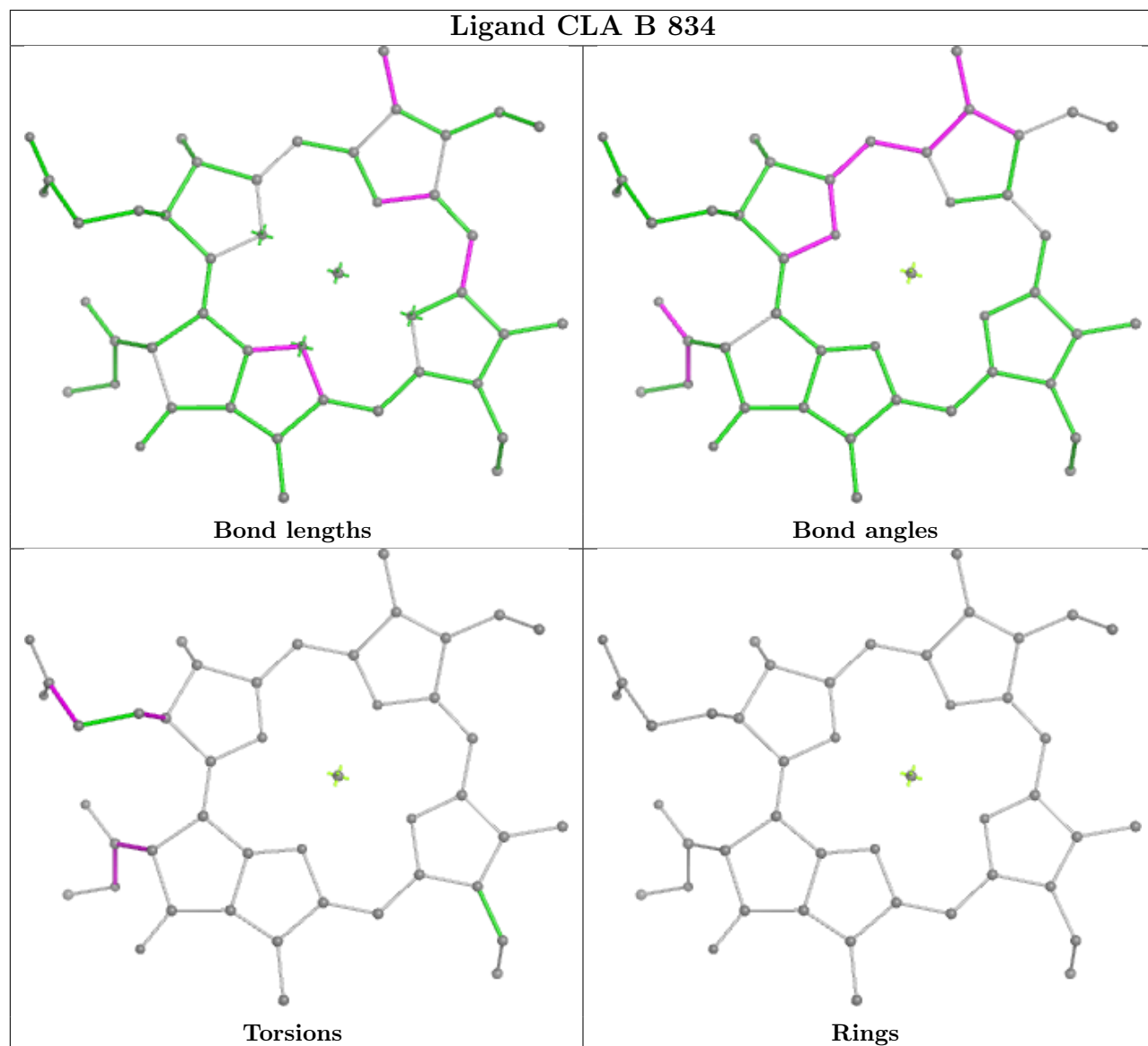






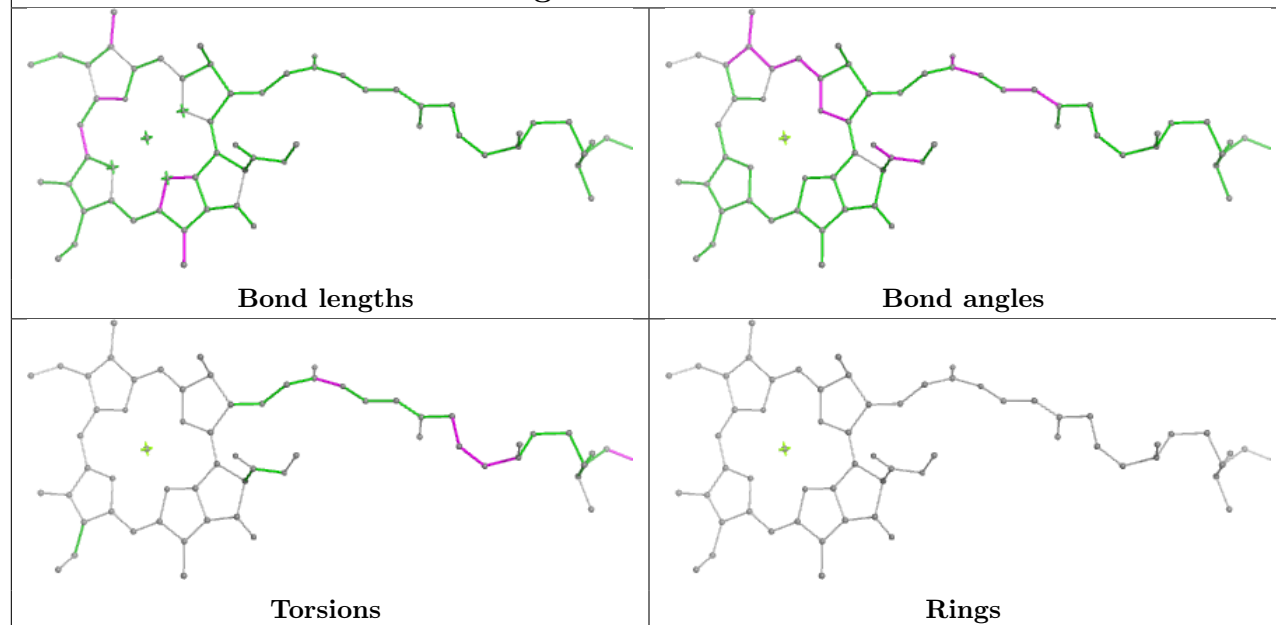


## Ligand CLA B 834

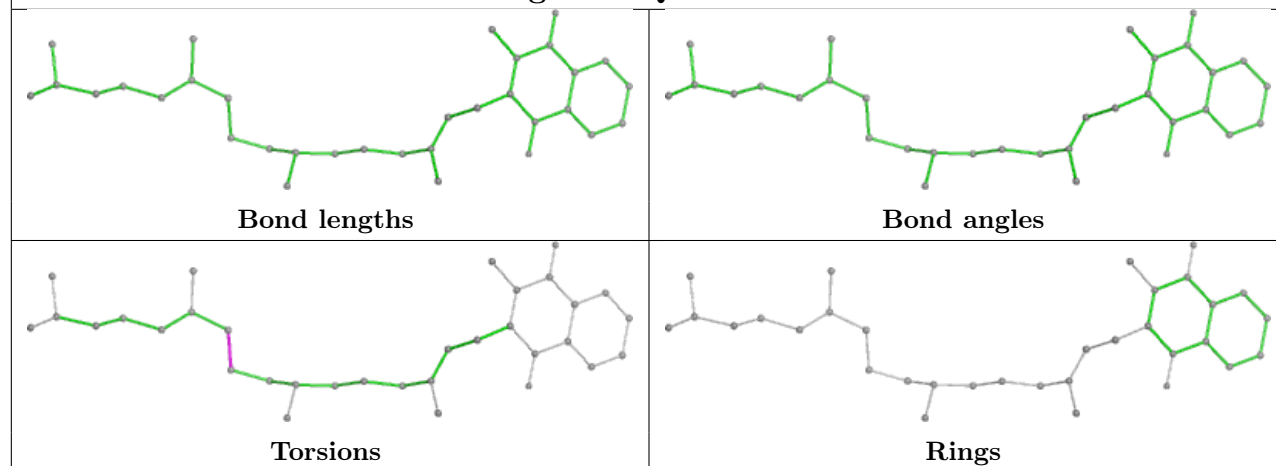




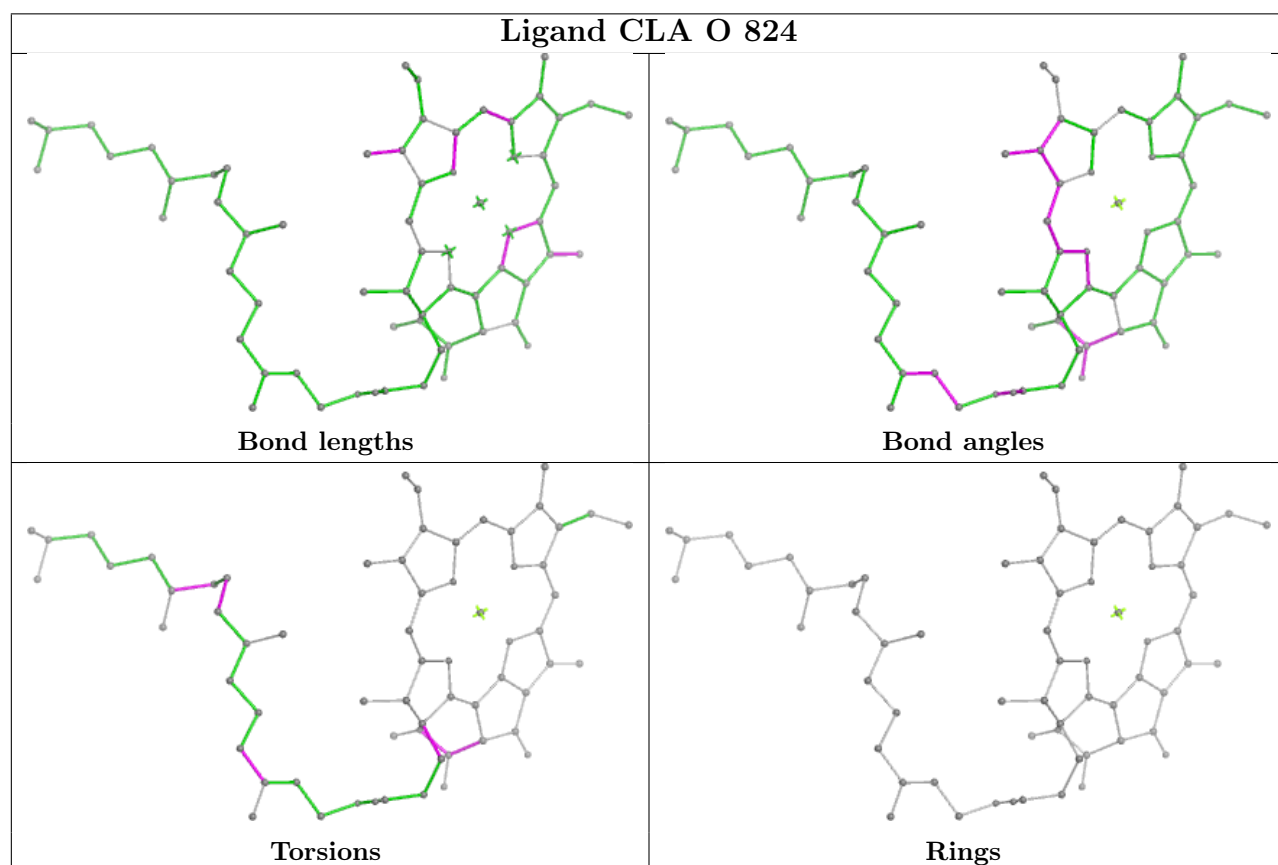
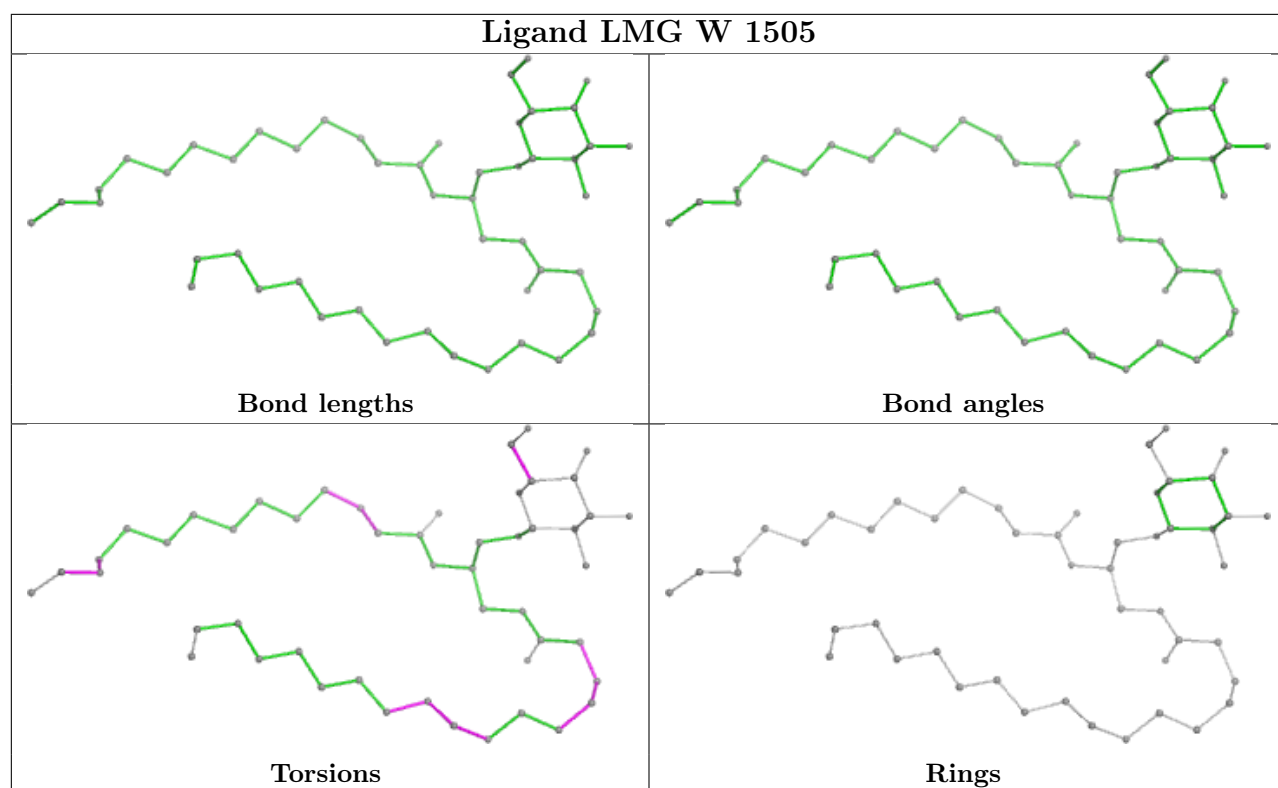
## Ligand CLA F 201



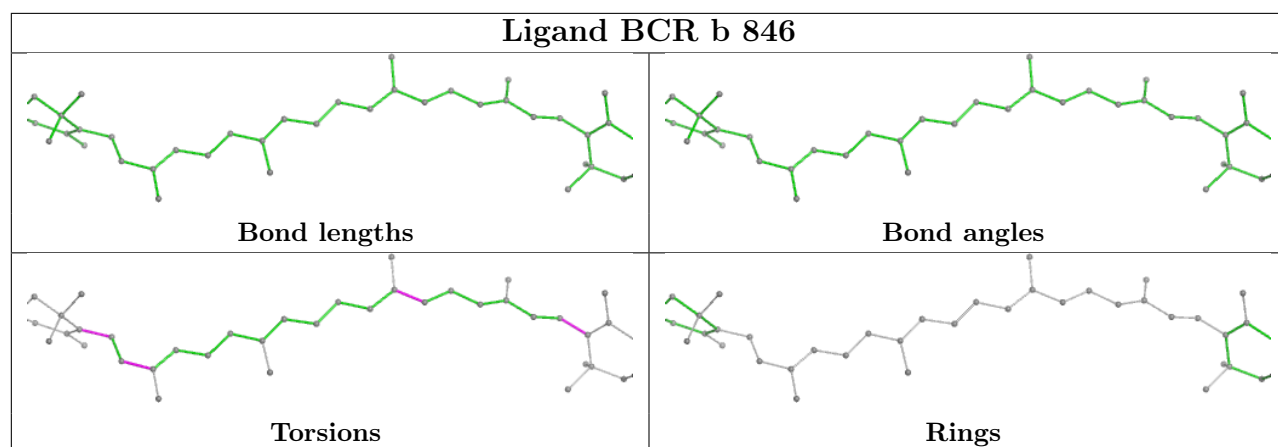
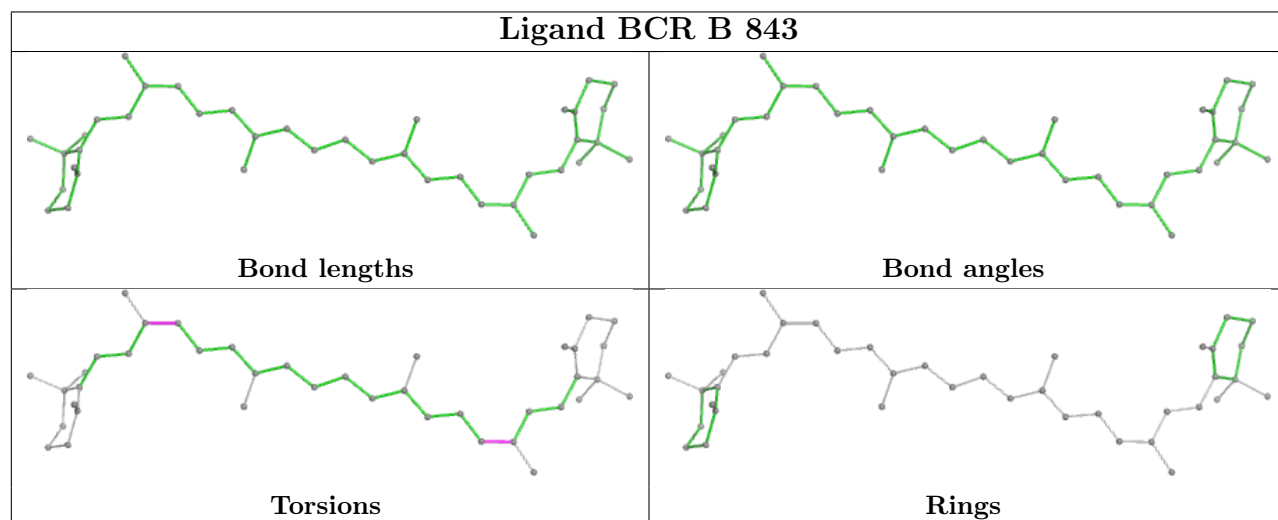
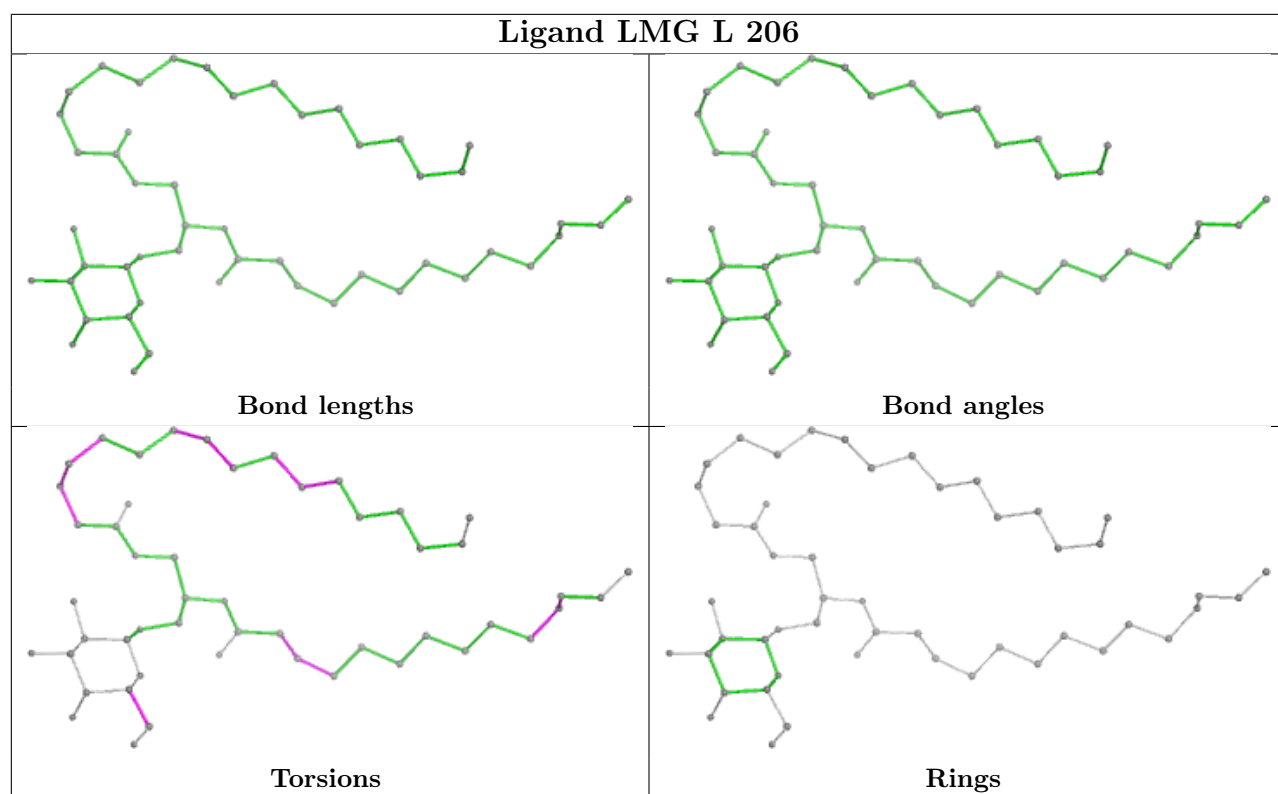
## Ligand PQN N 843



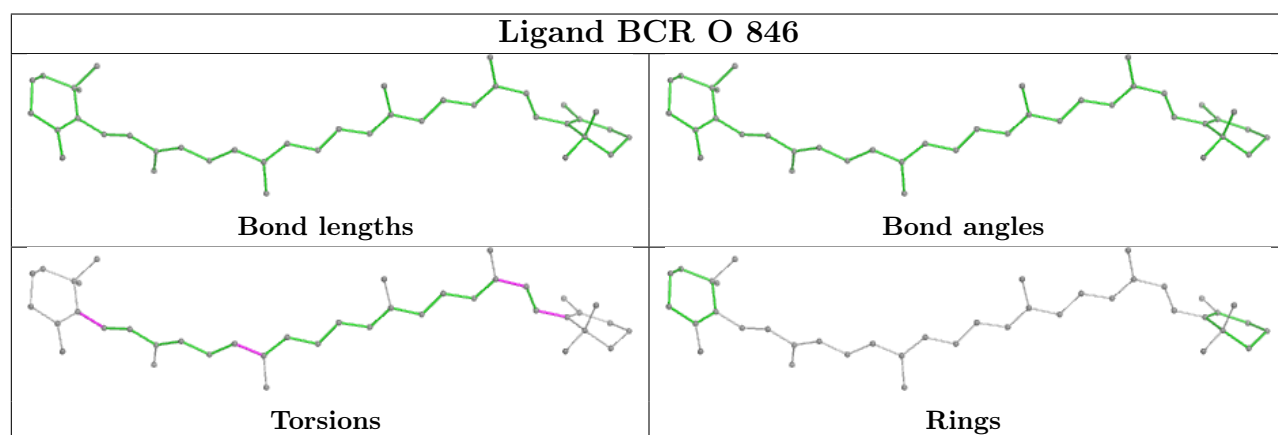
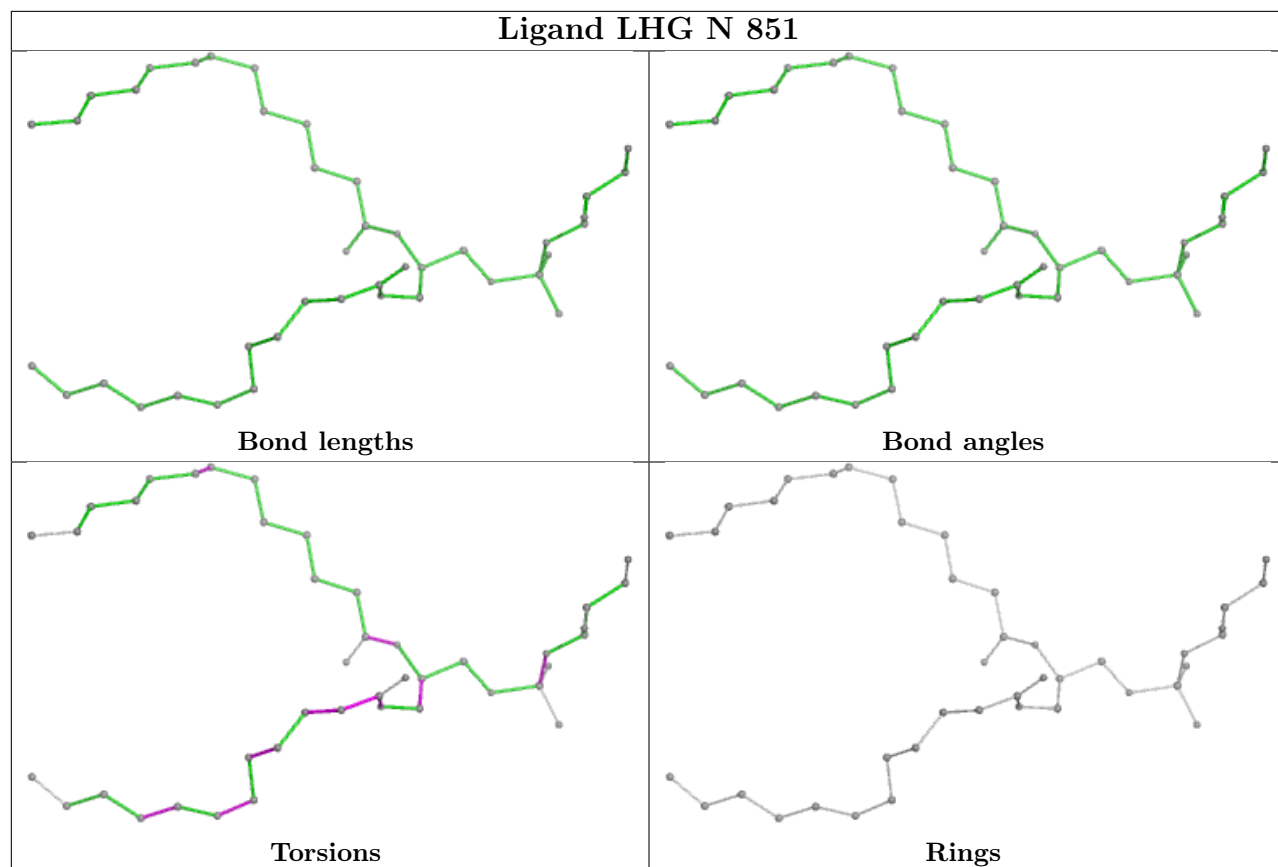




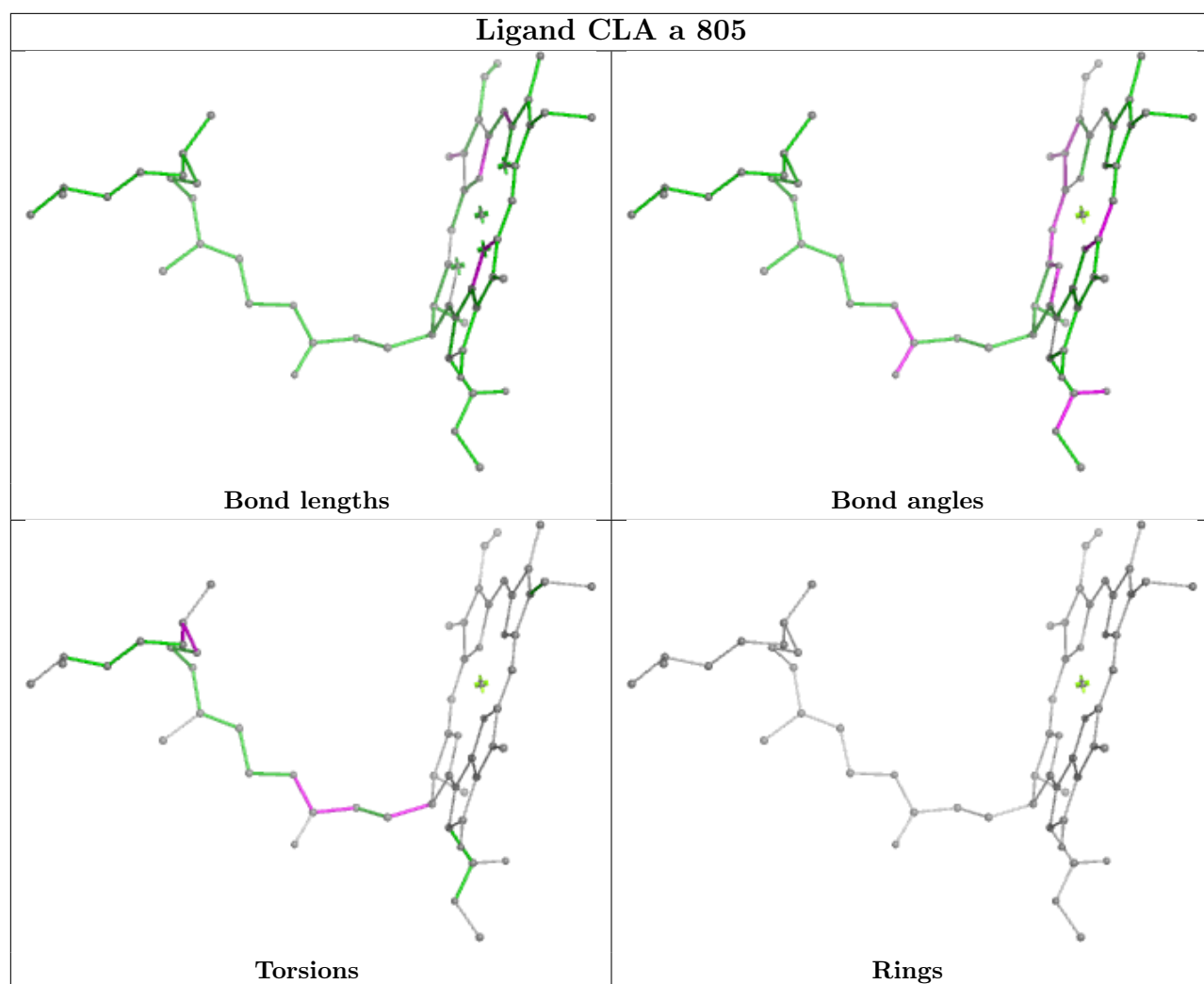






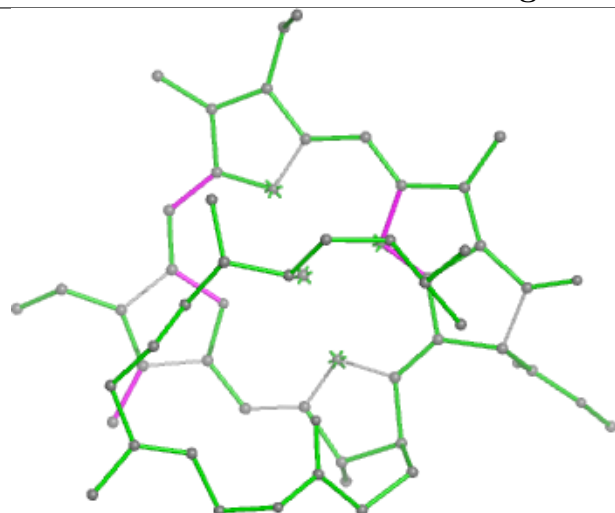




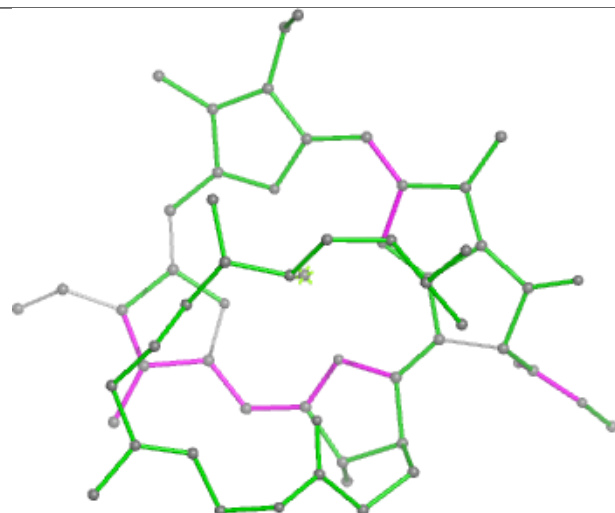




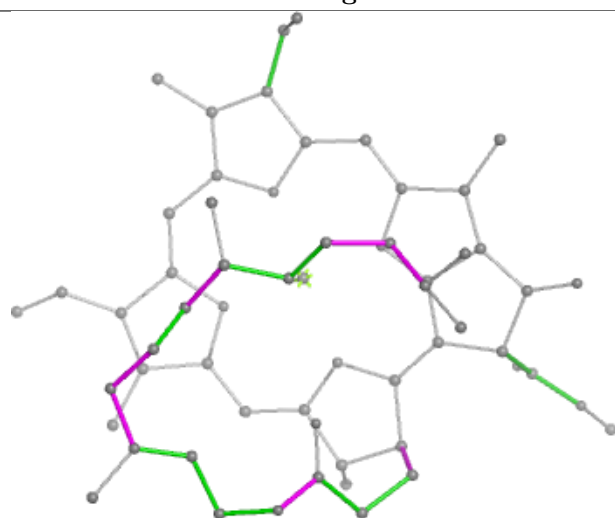
## Ligand CLA b 818



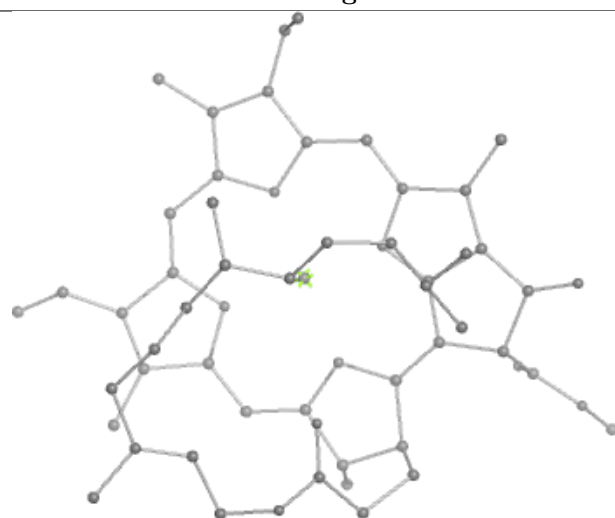
Bond lengths



Bond angles



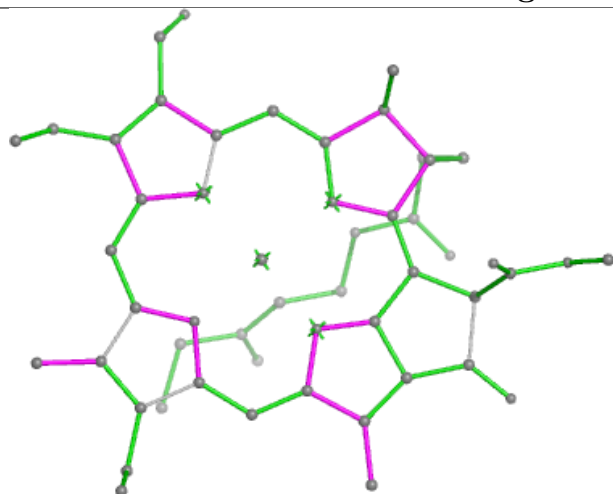
Torsions



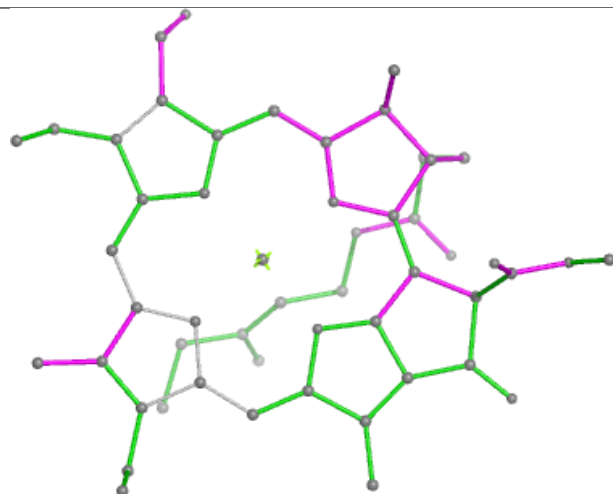
Rings



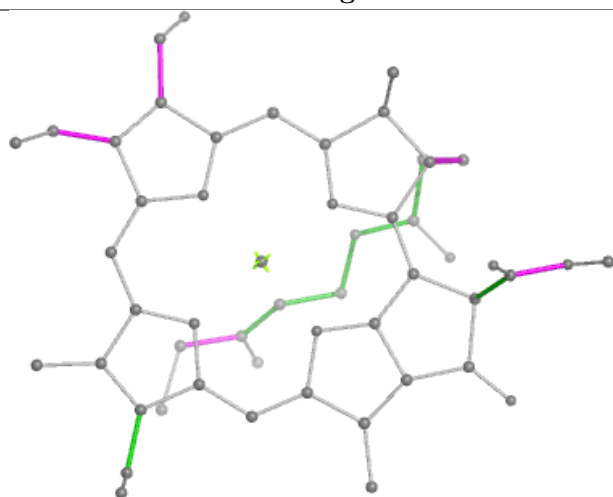
## Ligand F6C A 824



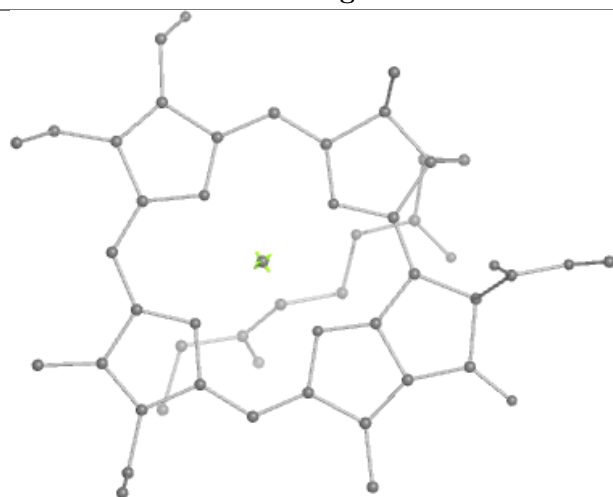
Bond lengths



Bond angles

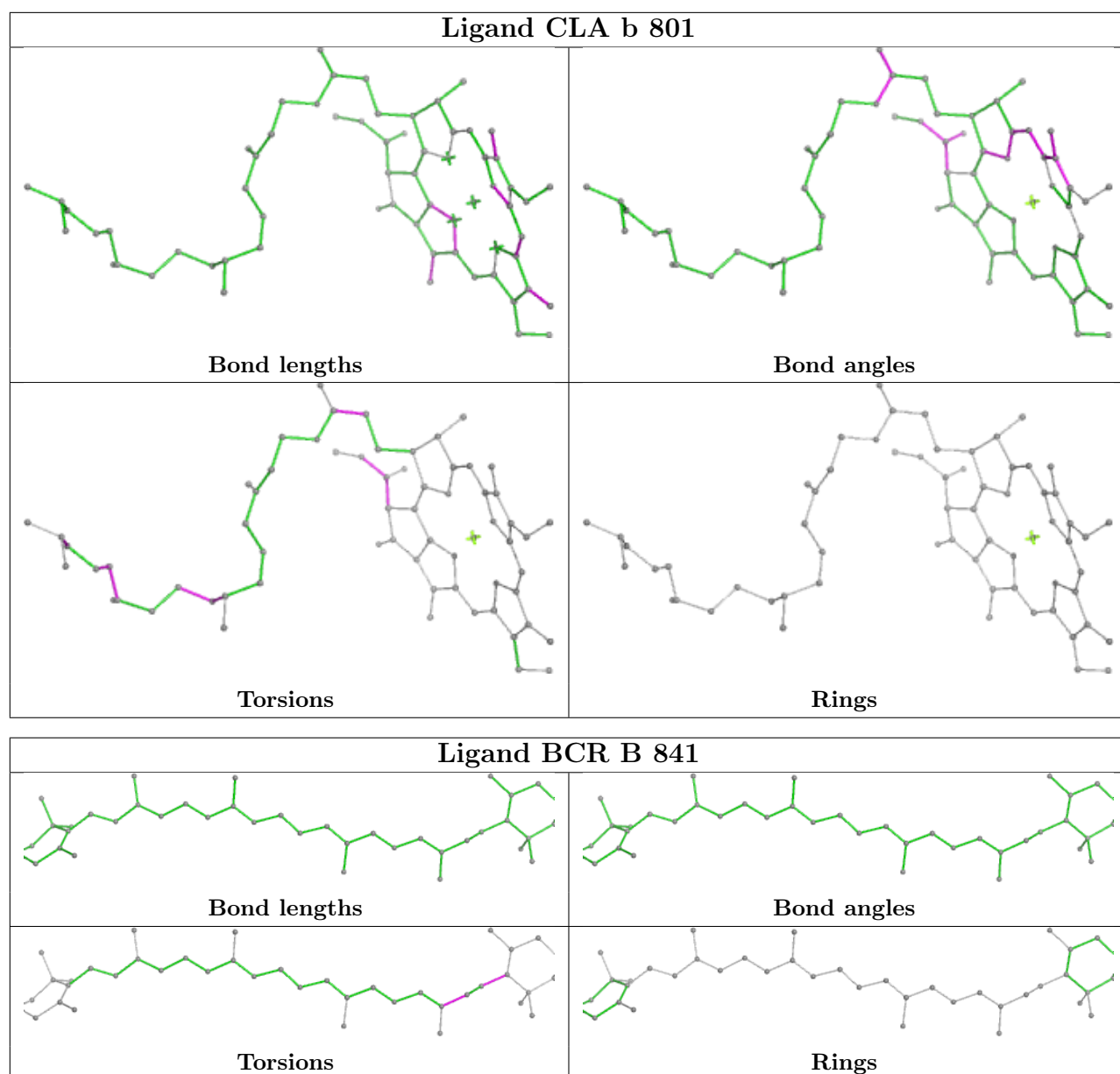


Torsions



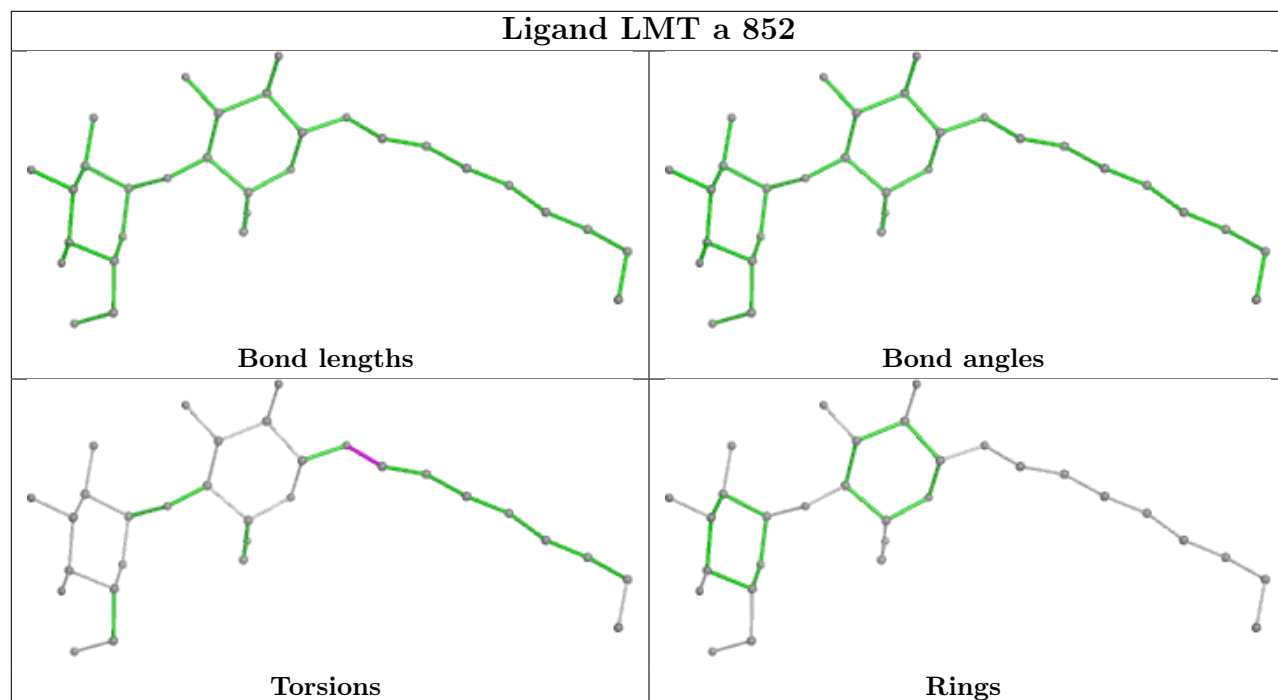
Rings



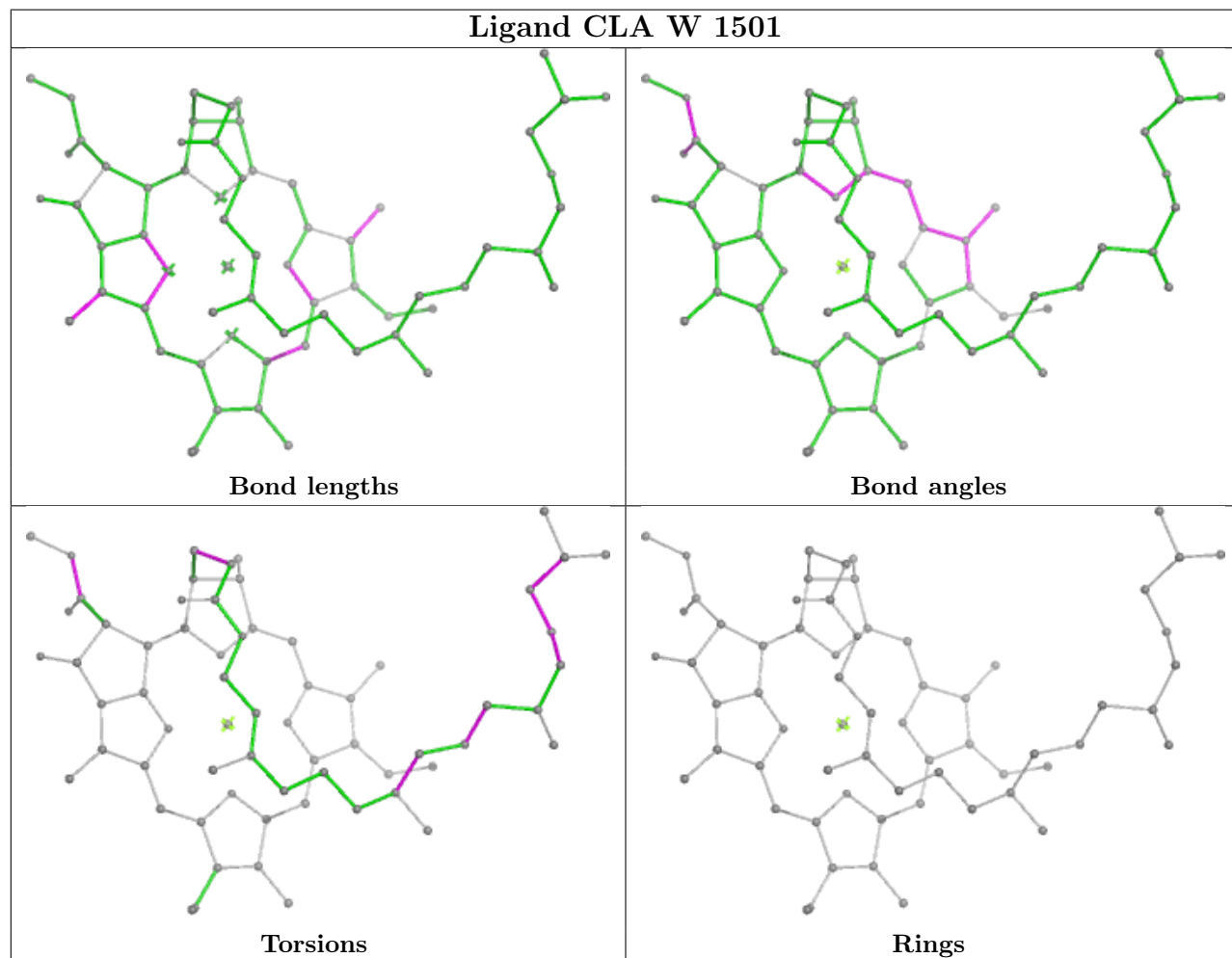




## Ligand LMT a 852

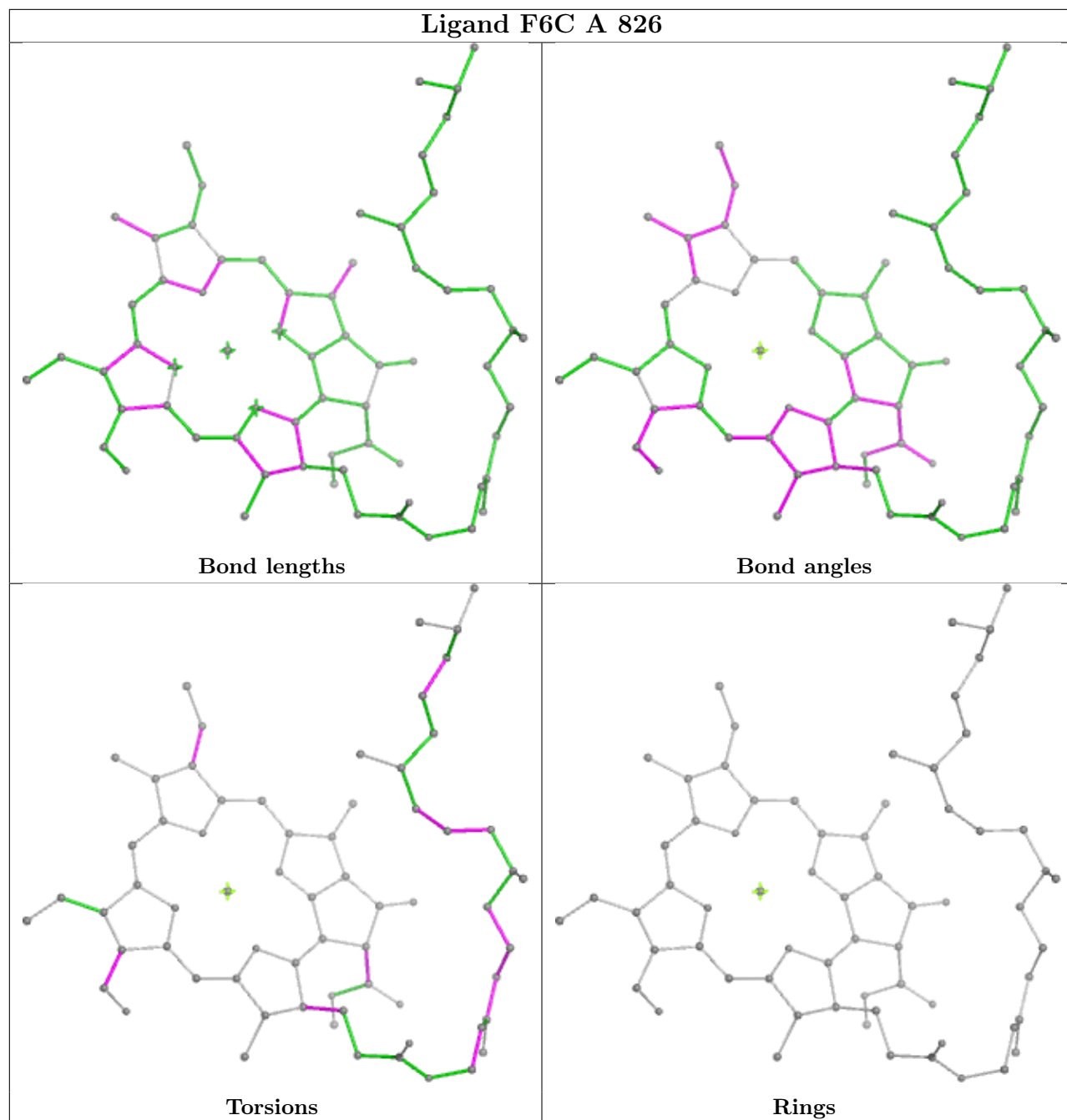


## Ligand CLA W 1501



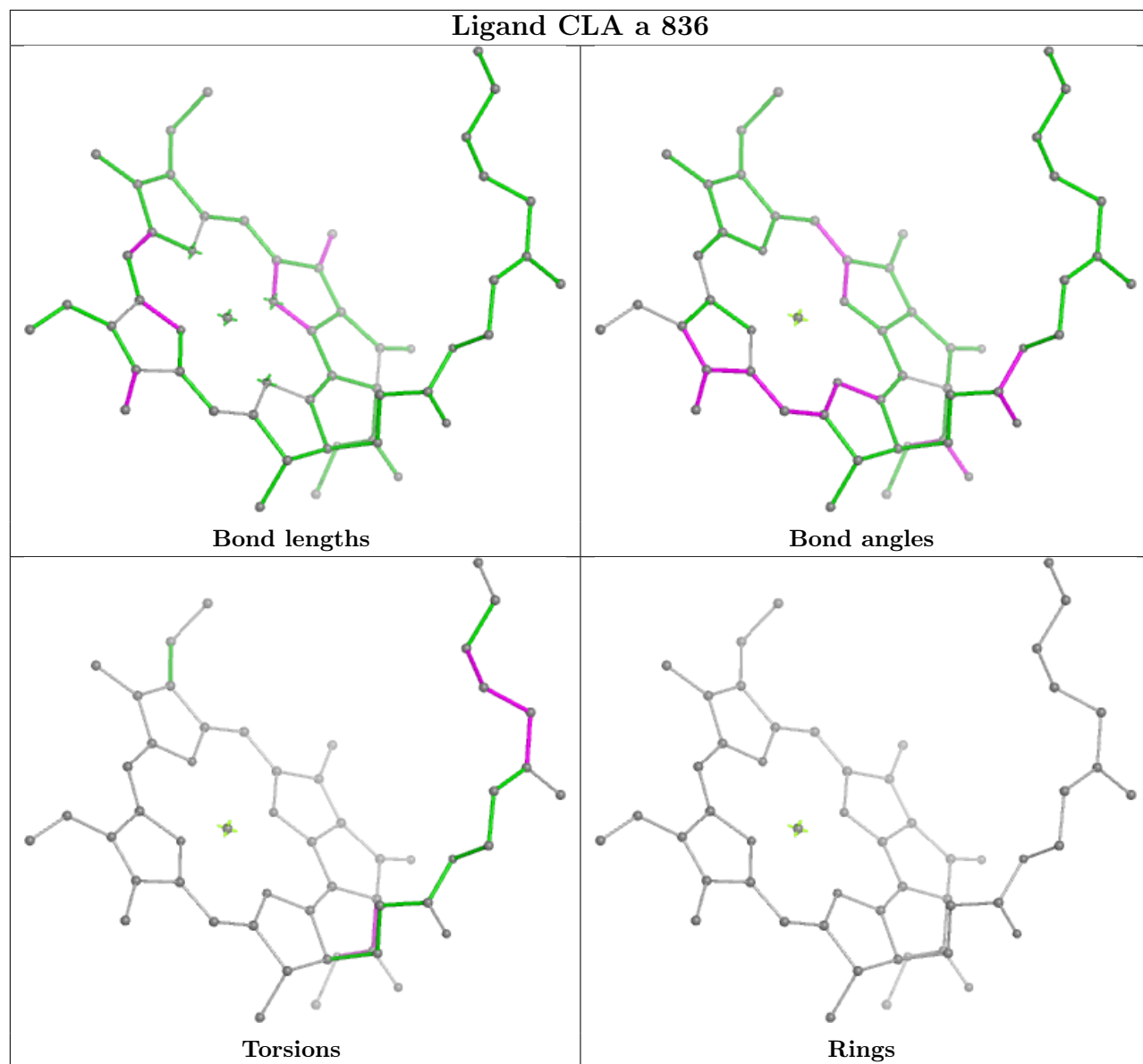


## Ligand F6C A 826

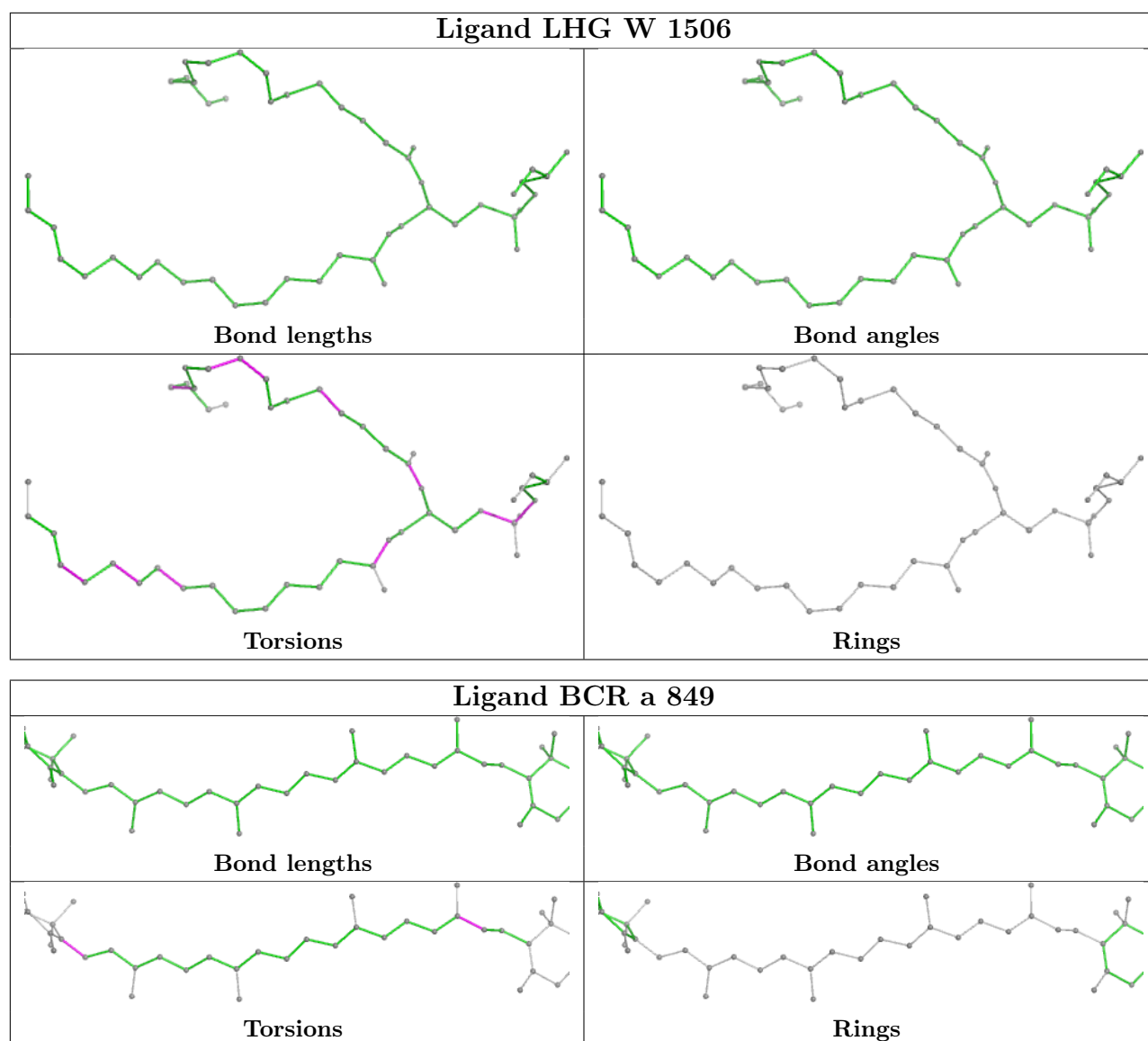




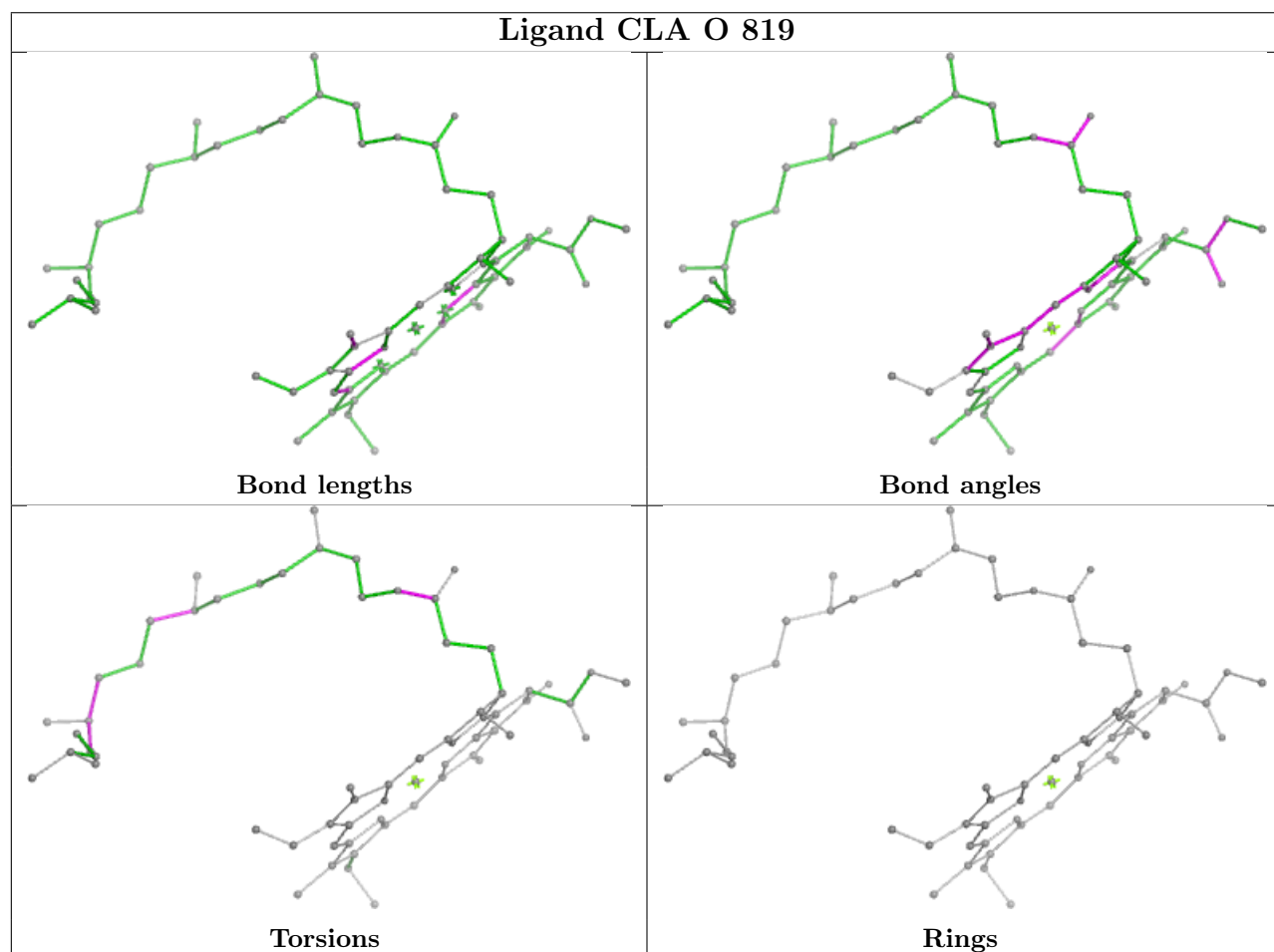
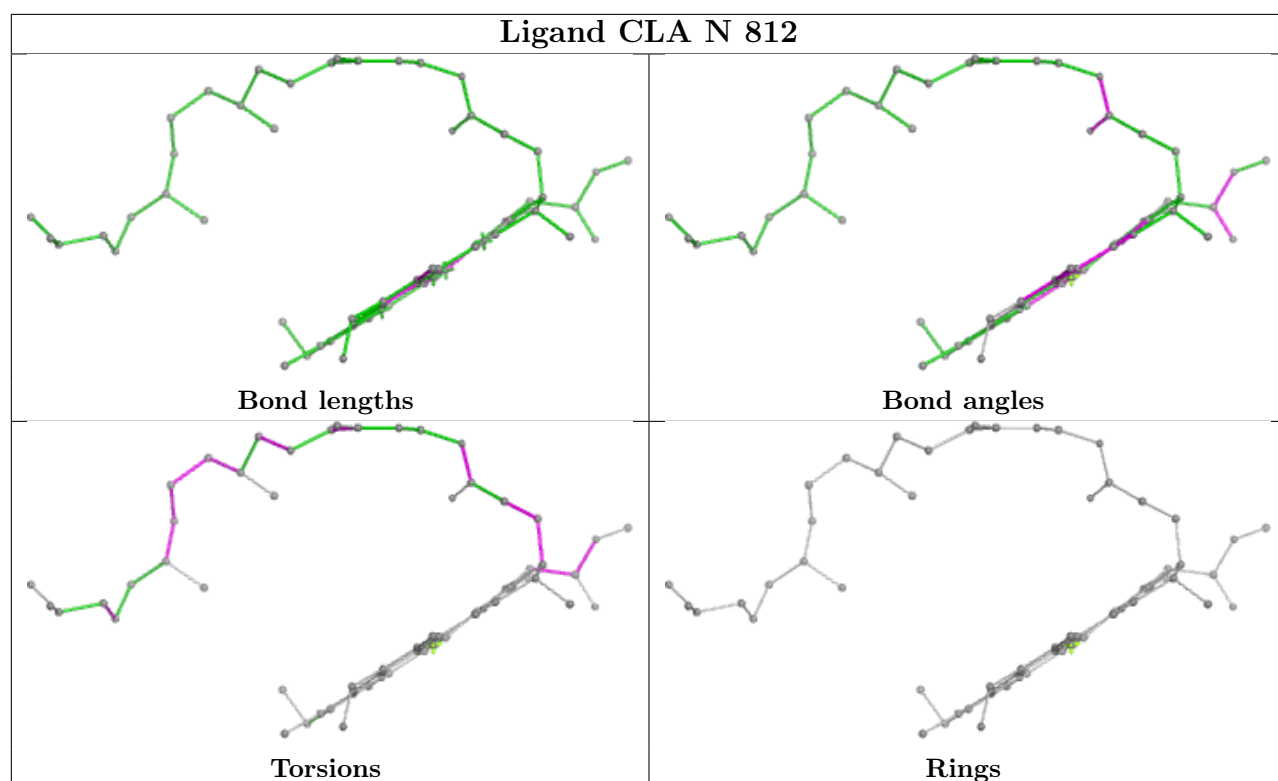
## Ligand CLA a 836



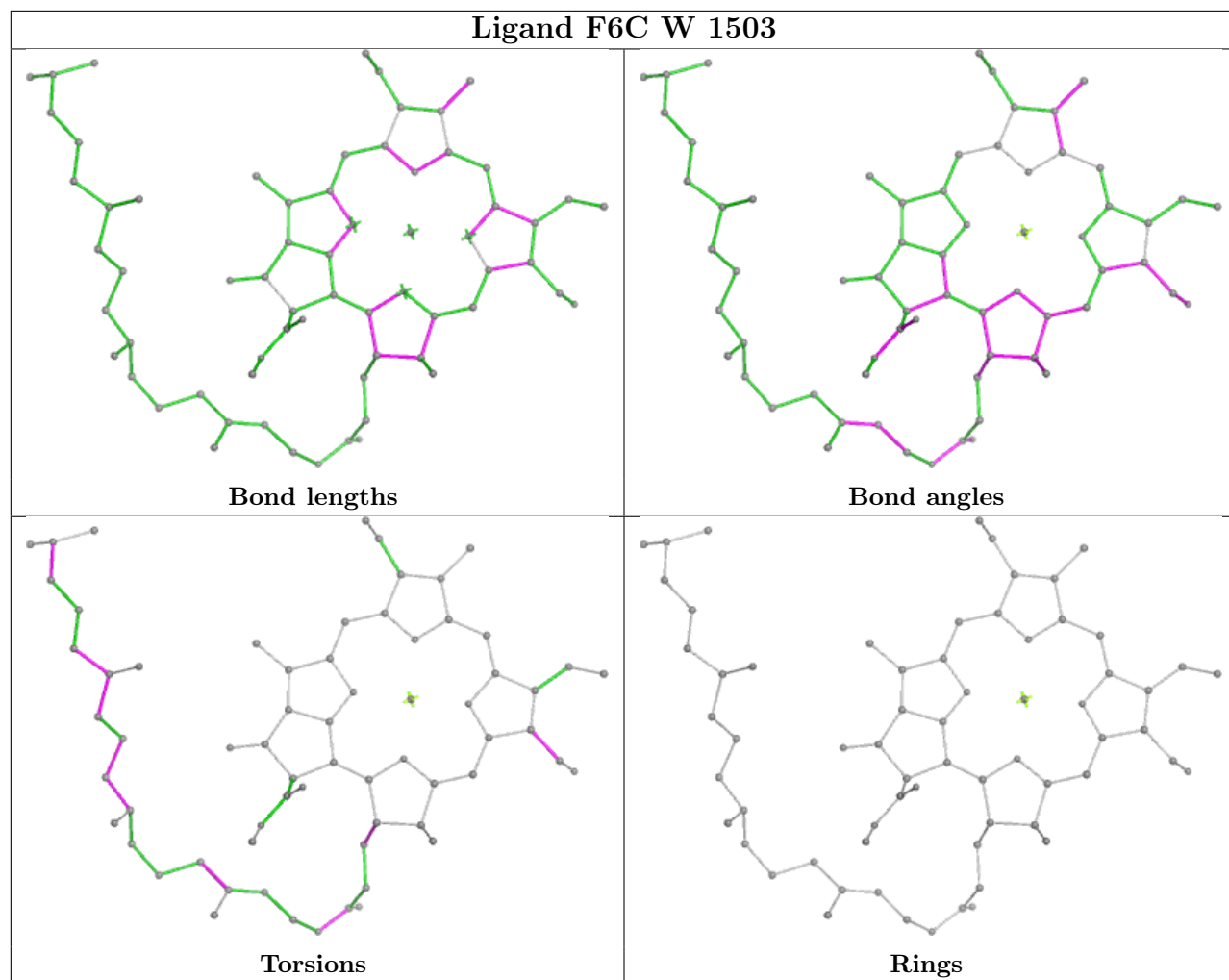






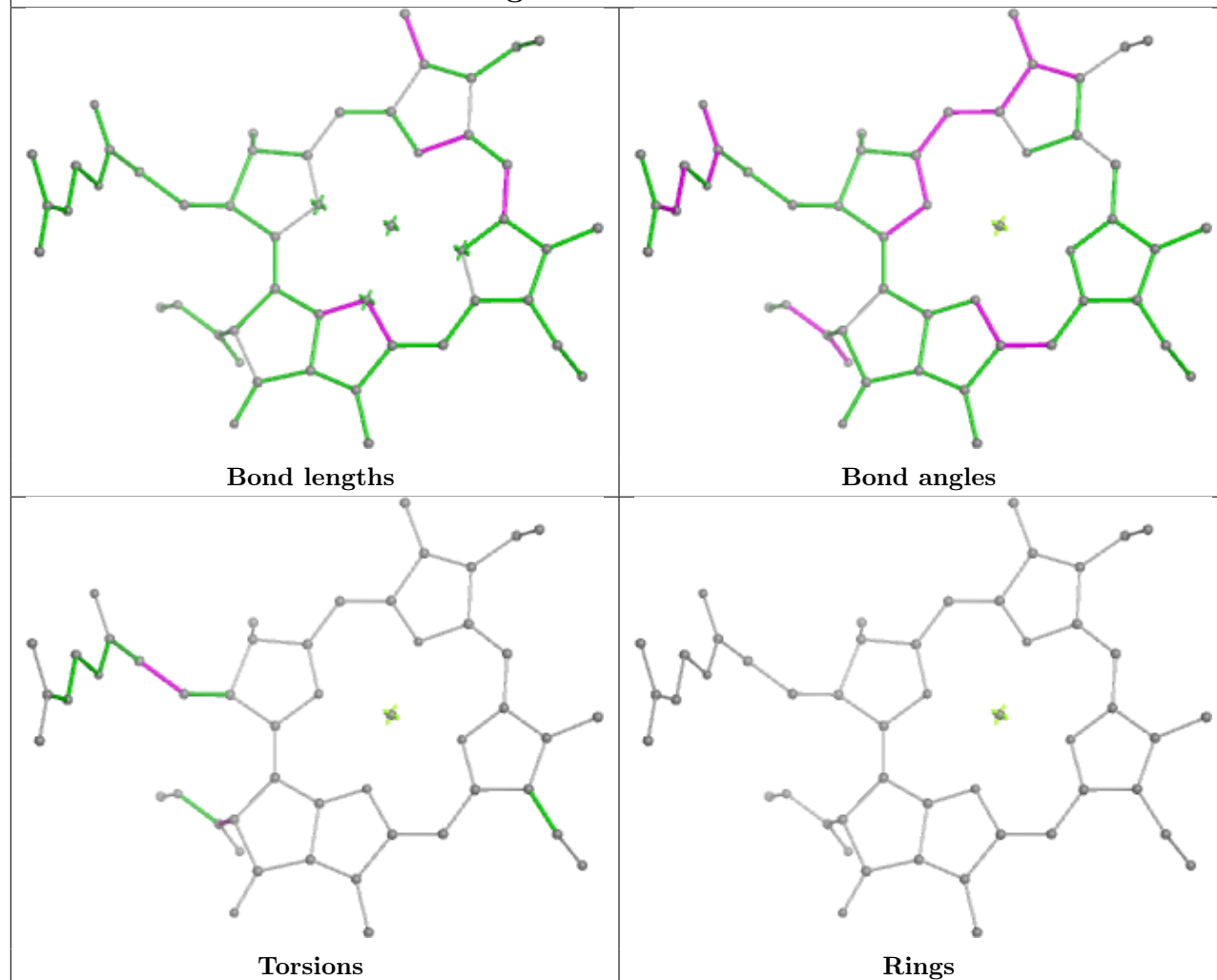




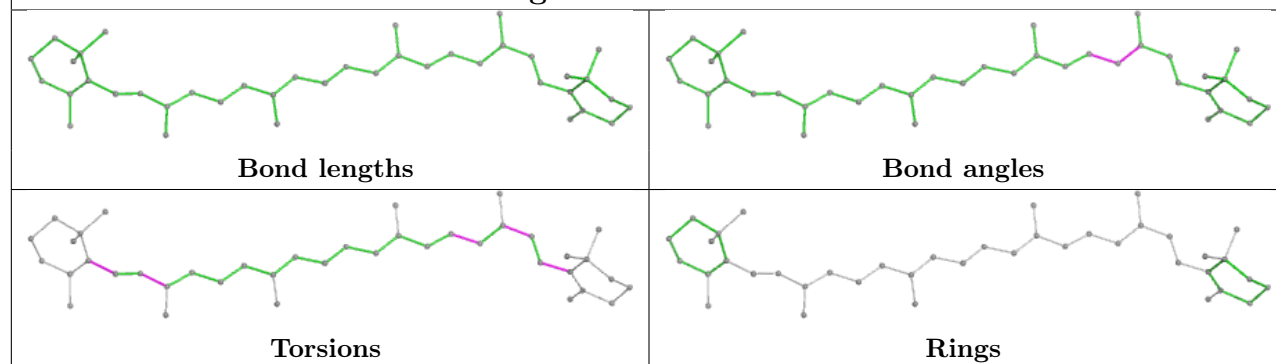




## Ligand CLA K 103

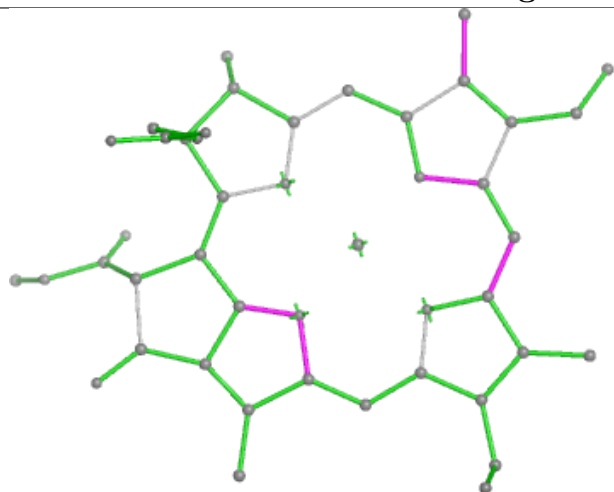


## Ligand BCR N 846

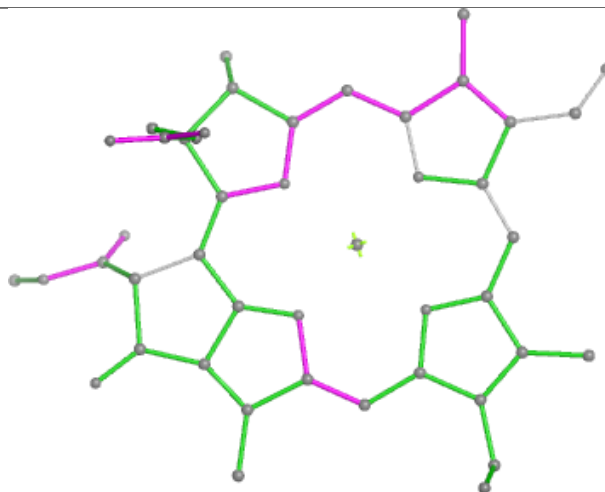




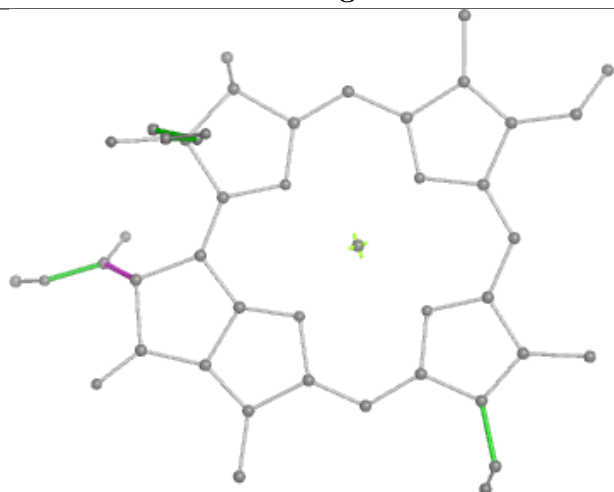
## Ligand CLA a 808



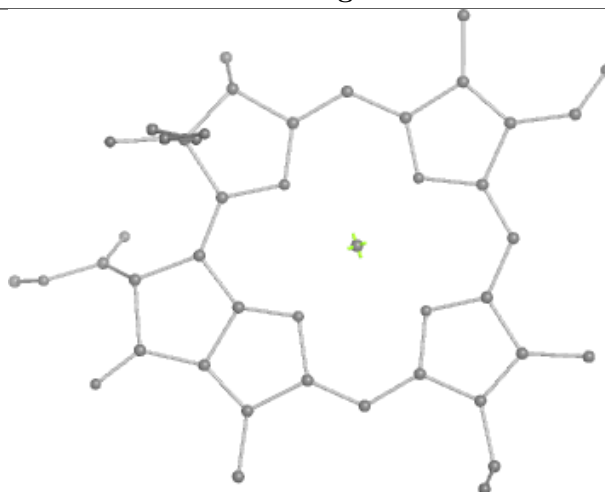
Bond lengths



Bond angles

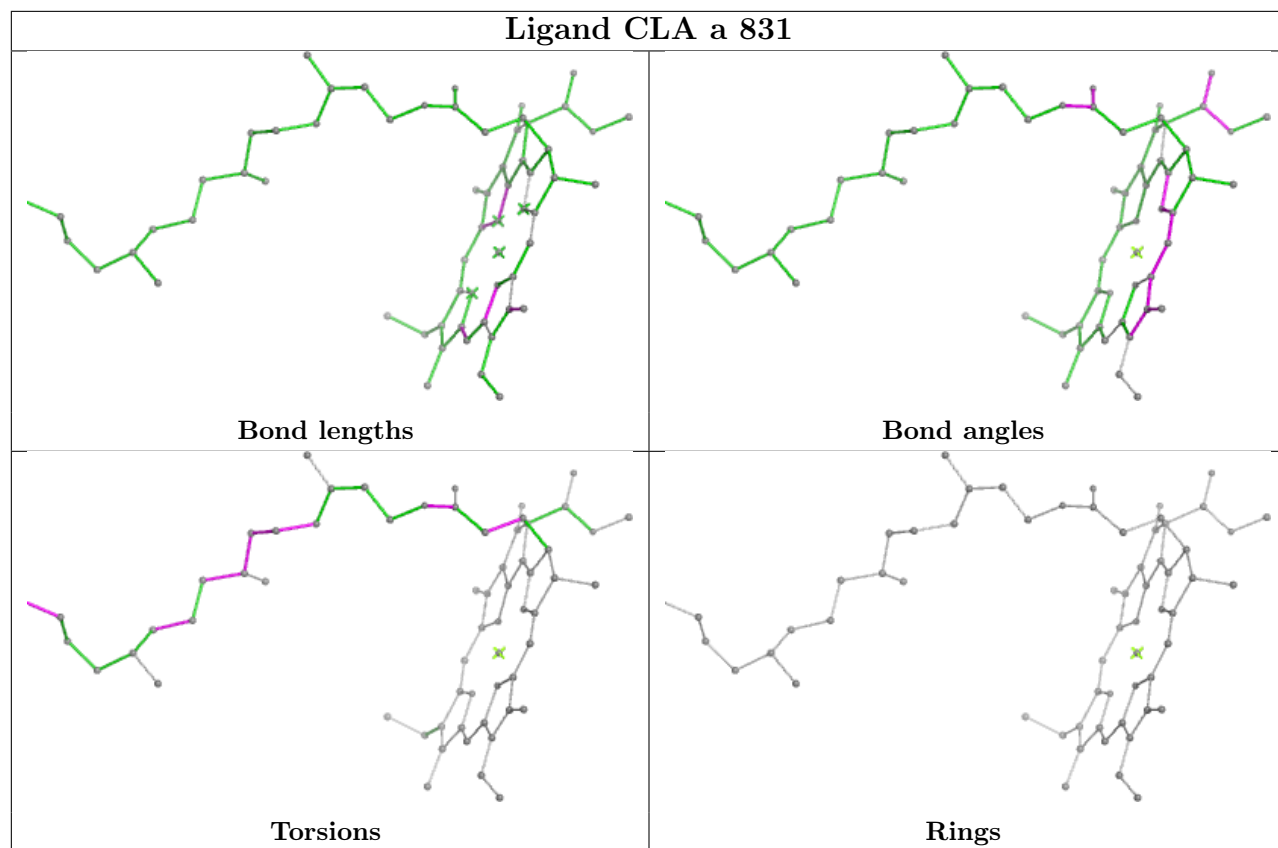


Torsions

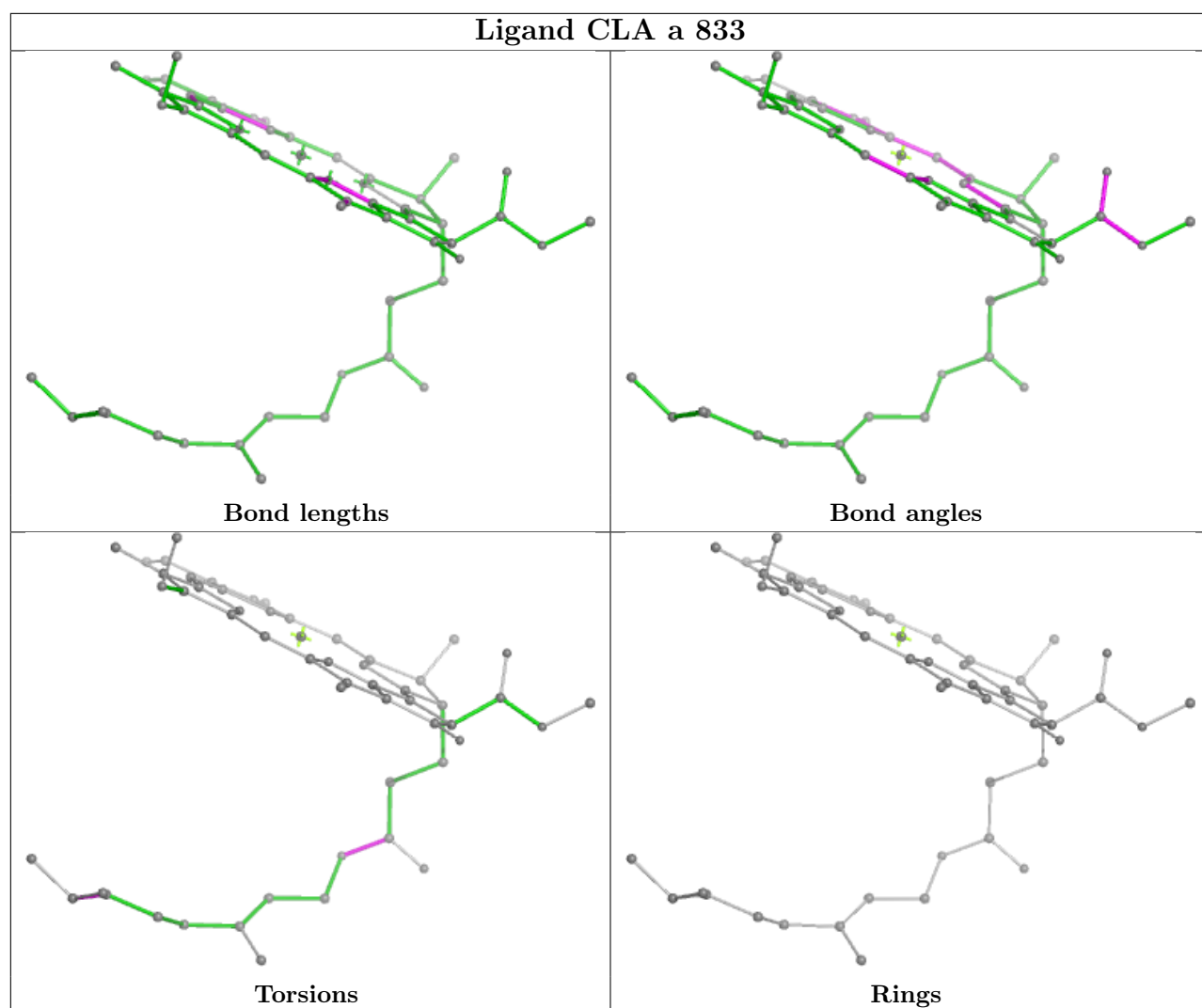


Rings

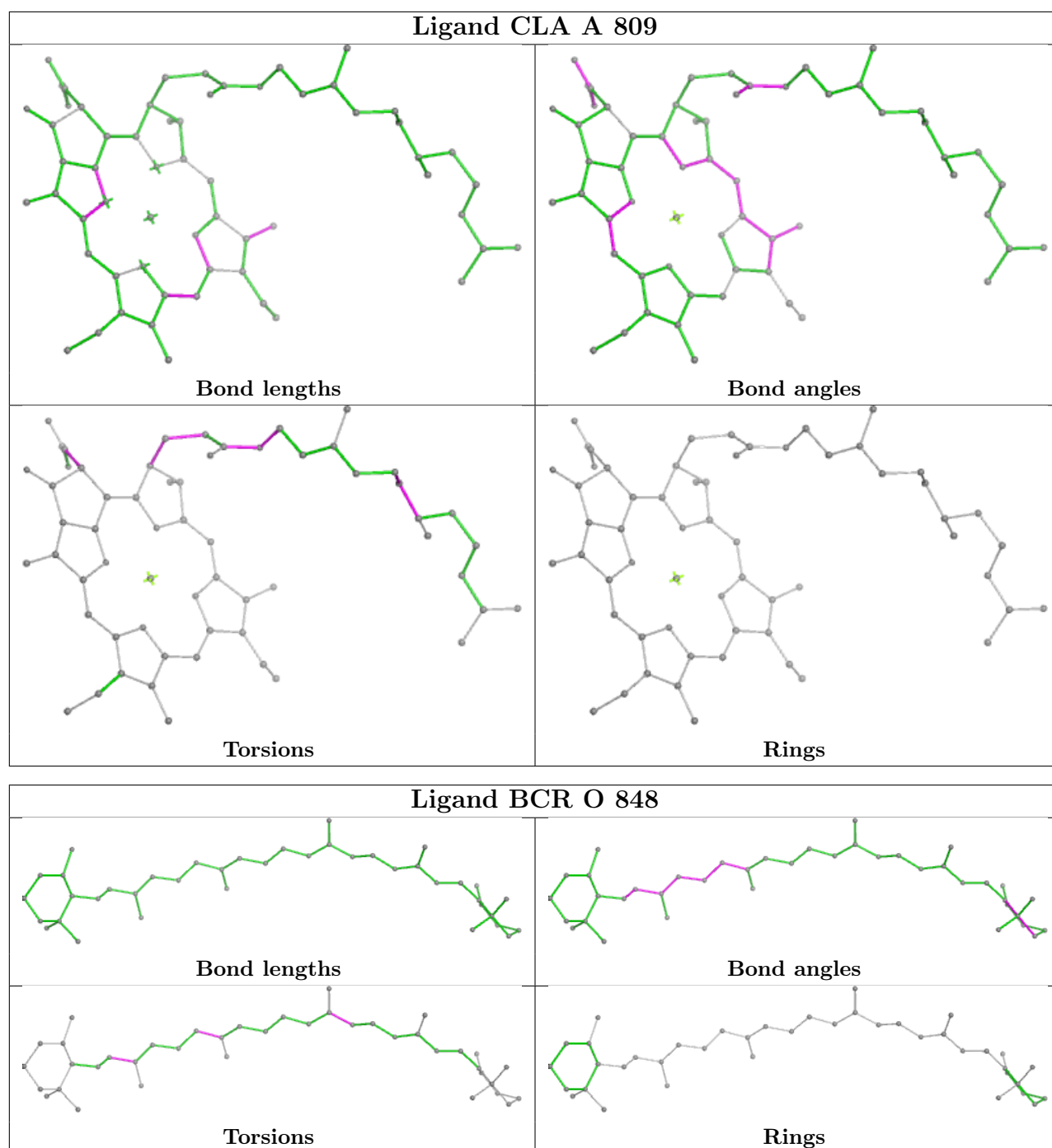






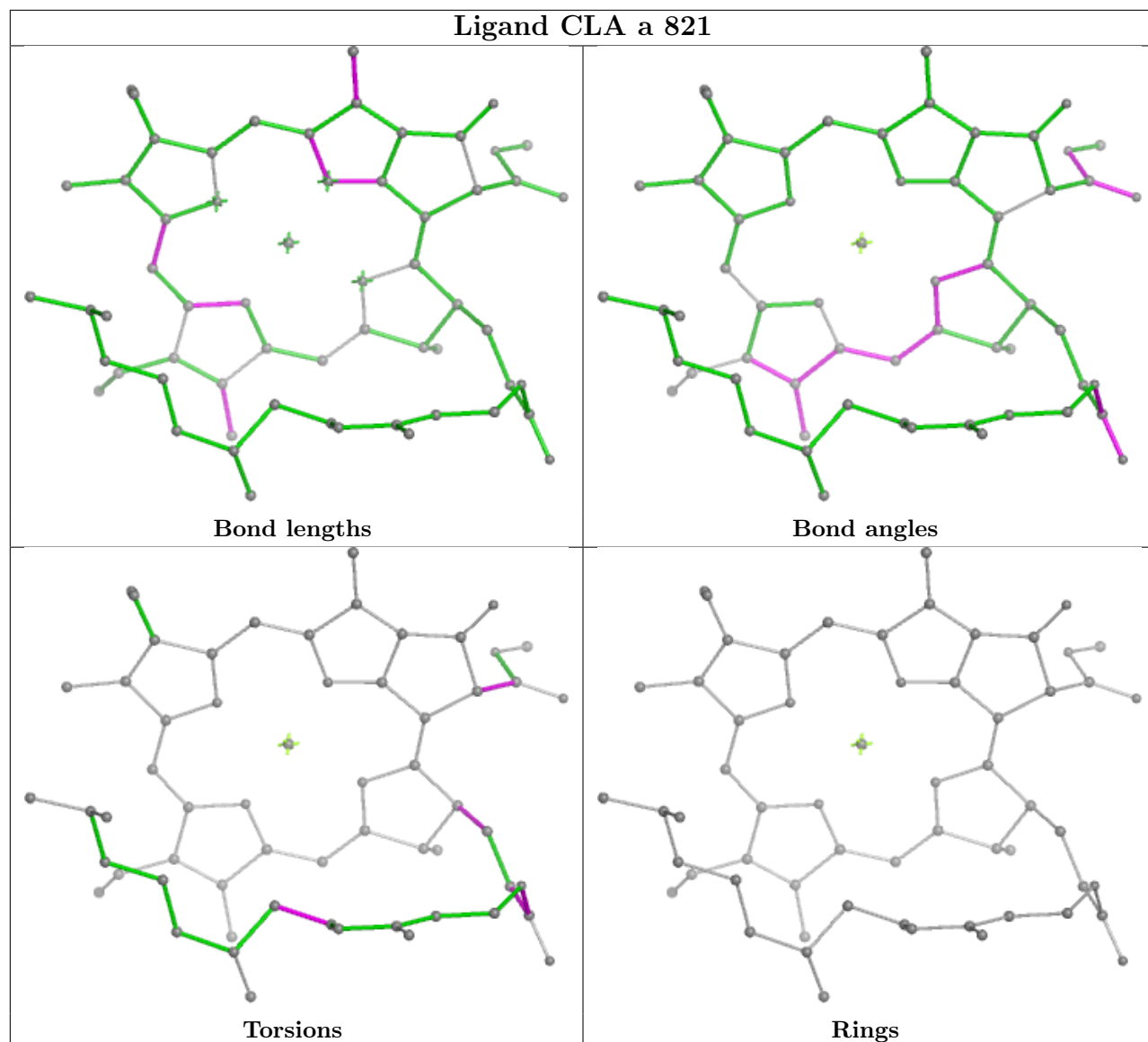




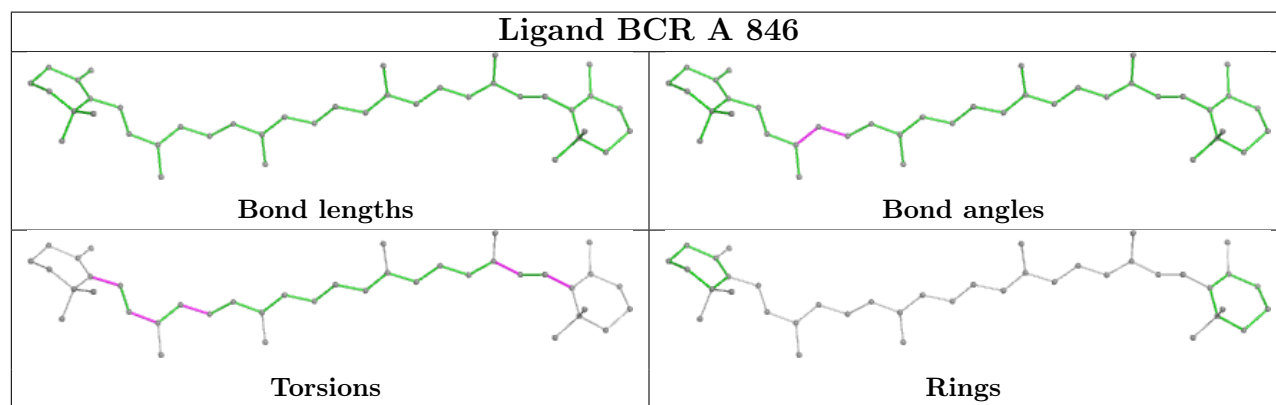
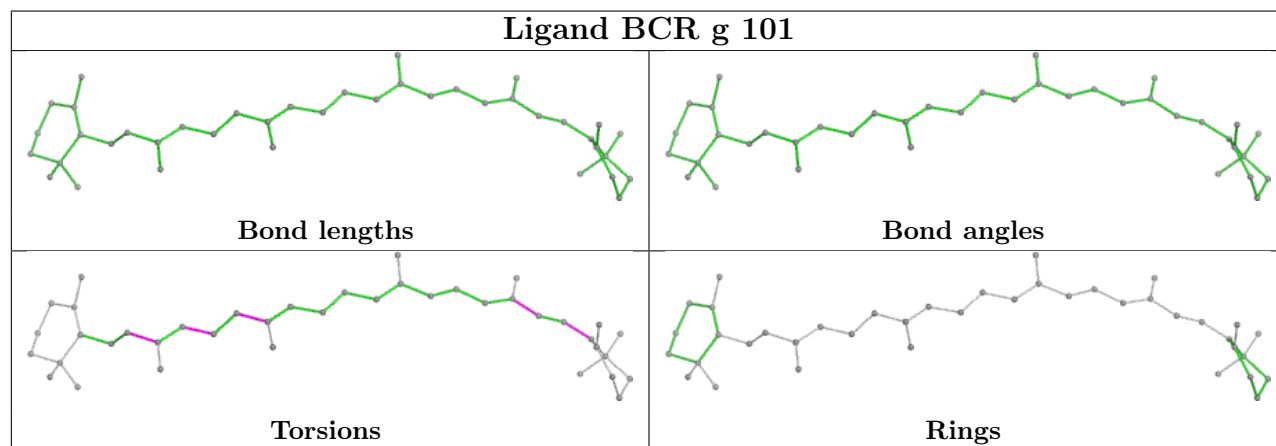
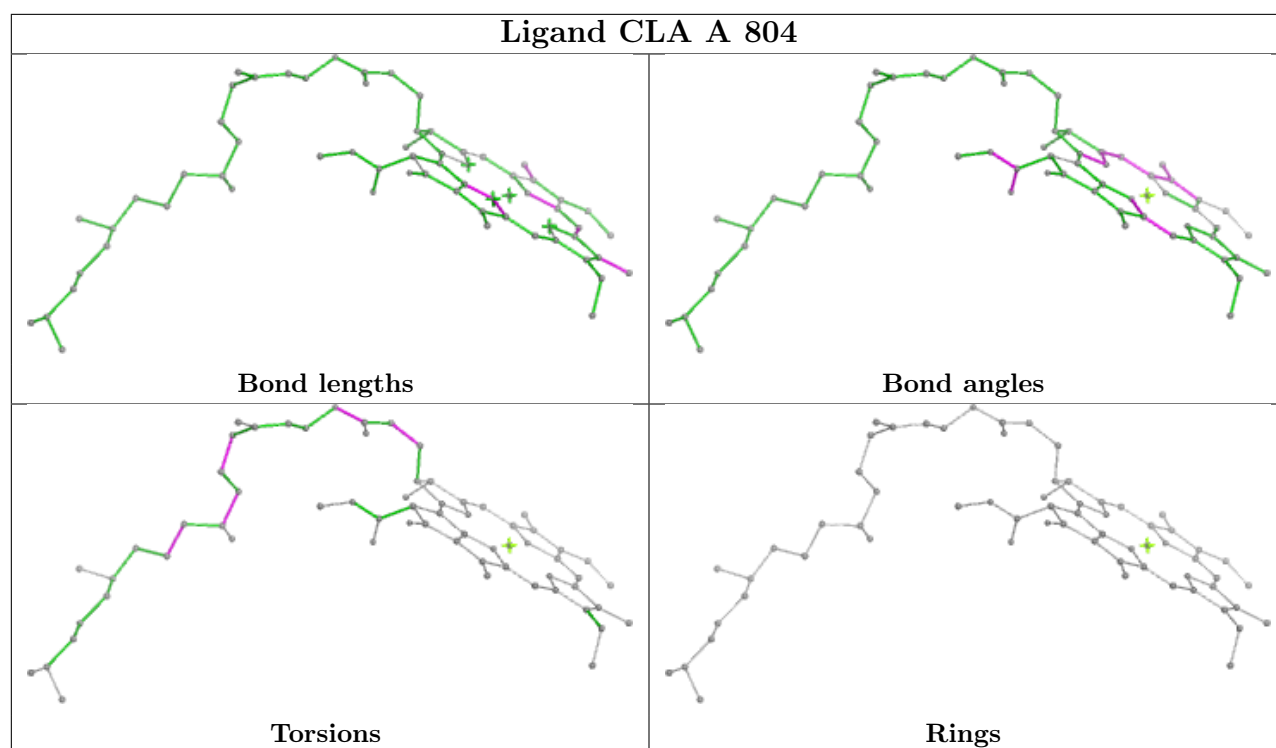




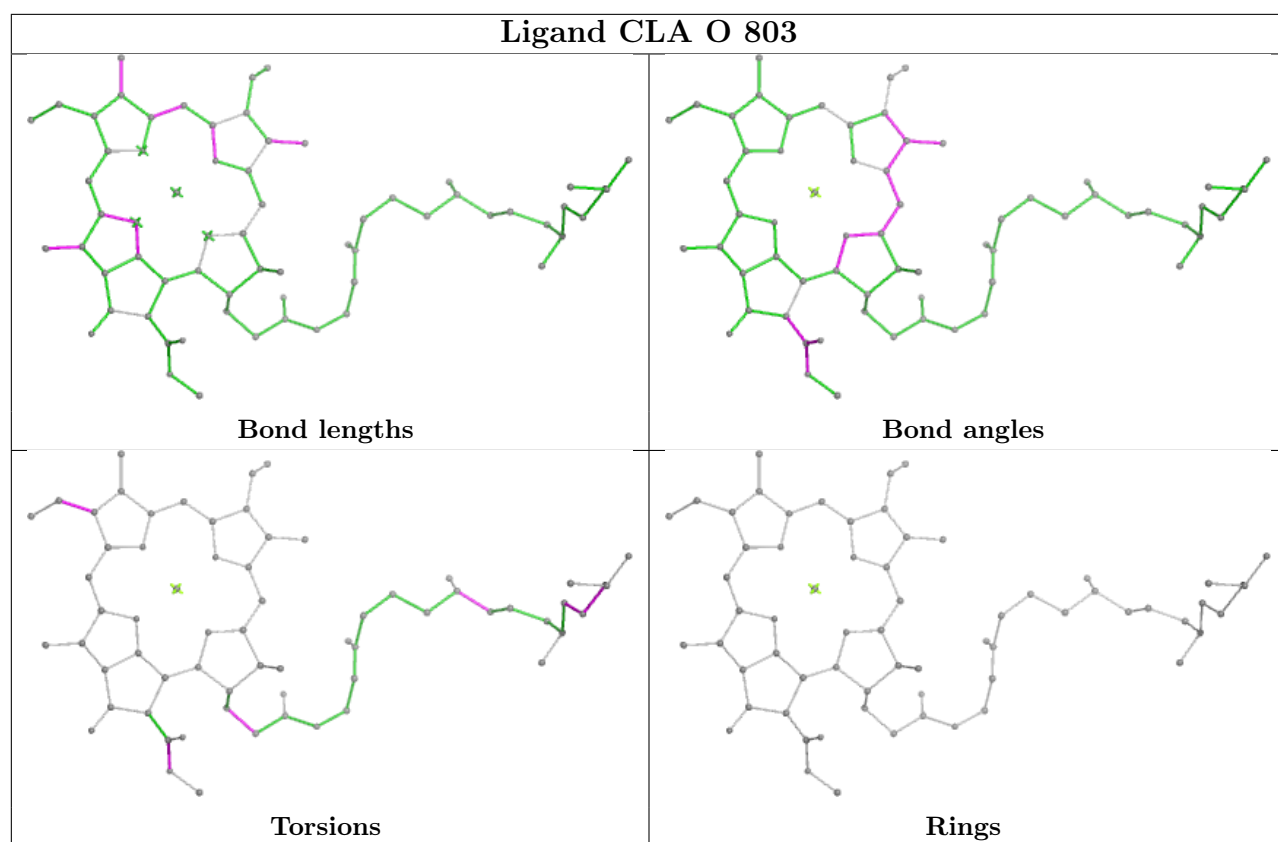
## Ligand CLA a 821





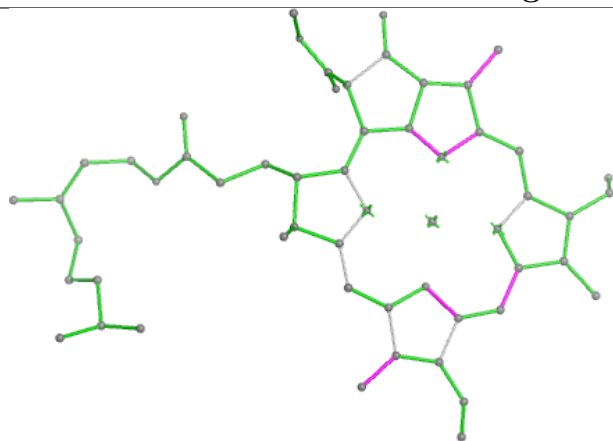




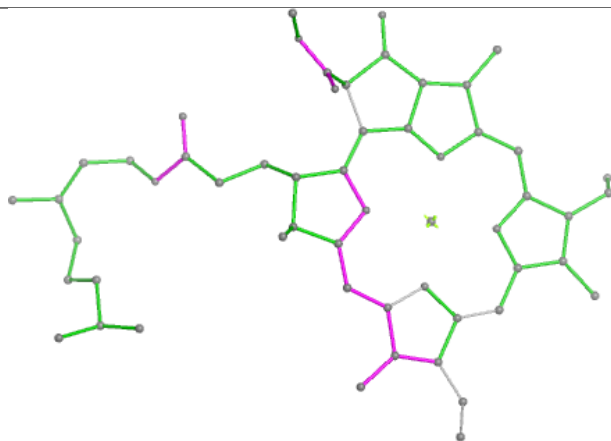




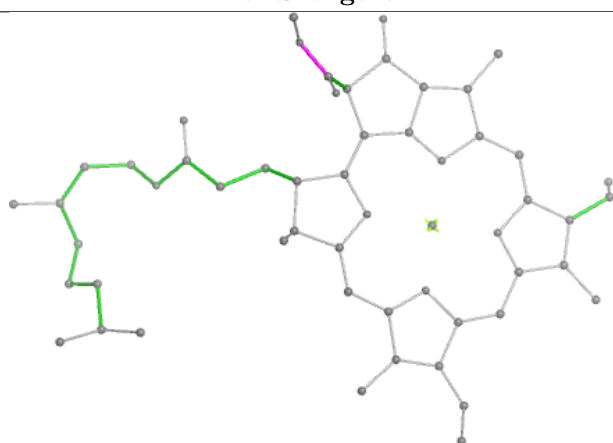
## Ligand CLA I 103



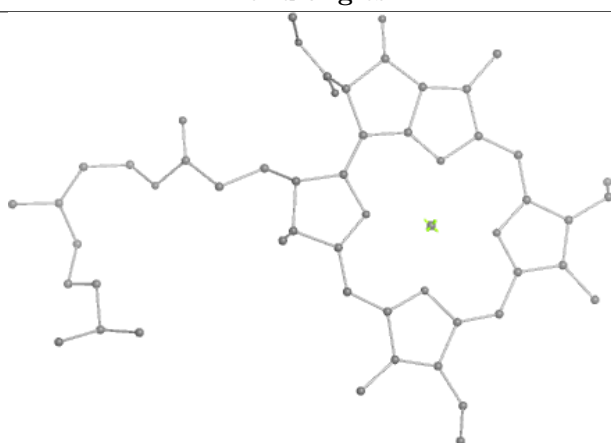
Bond lengths



Bond angles

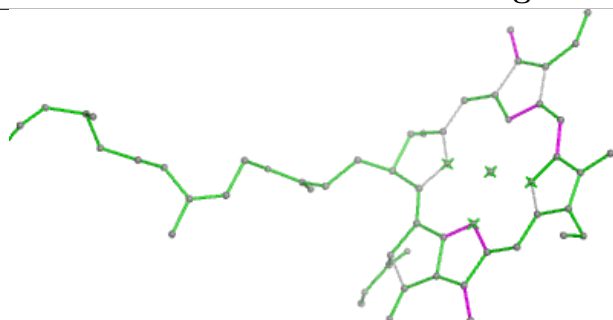


Torsions

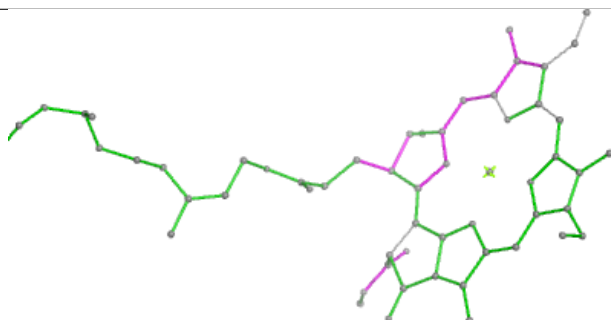


Rings

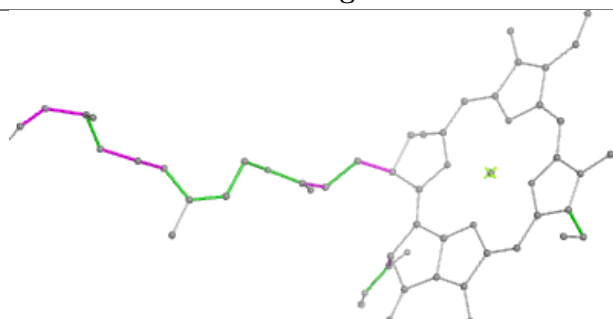
## Ligand CLA N 810



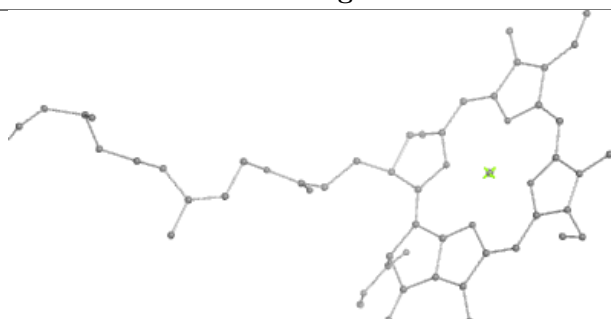
Bond lengths



Bond angles



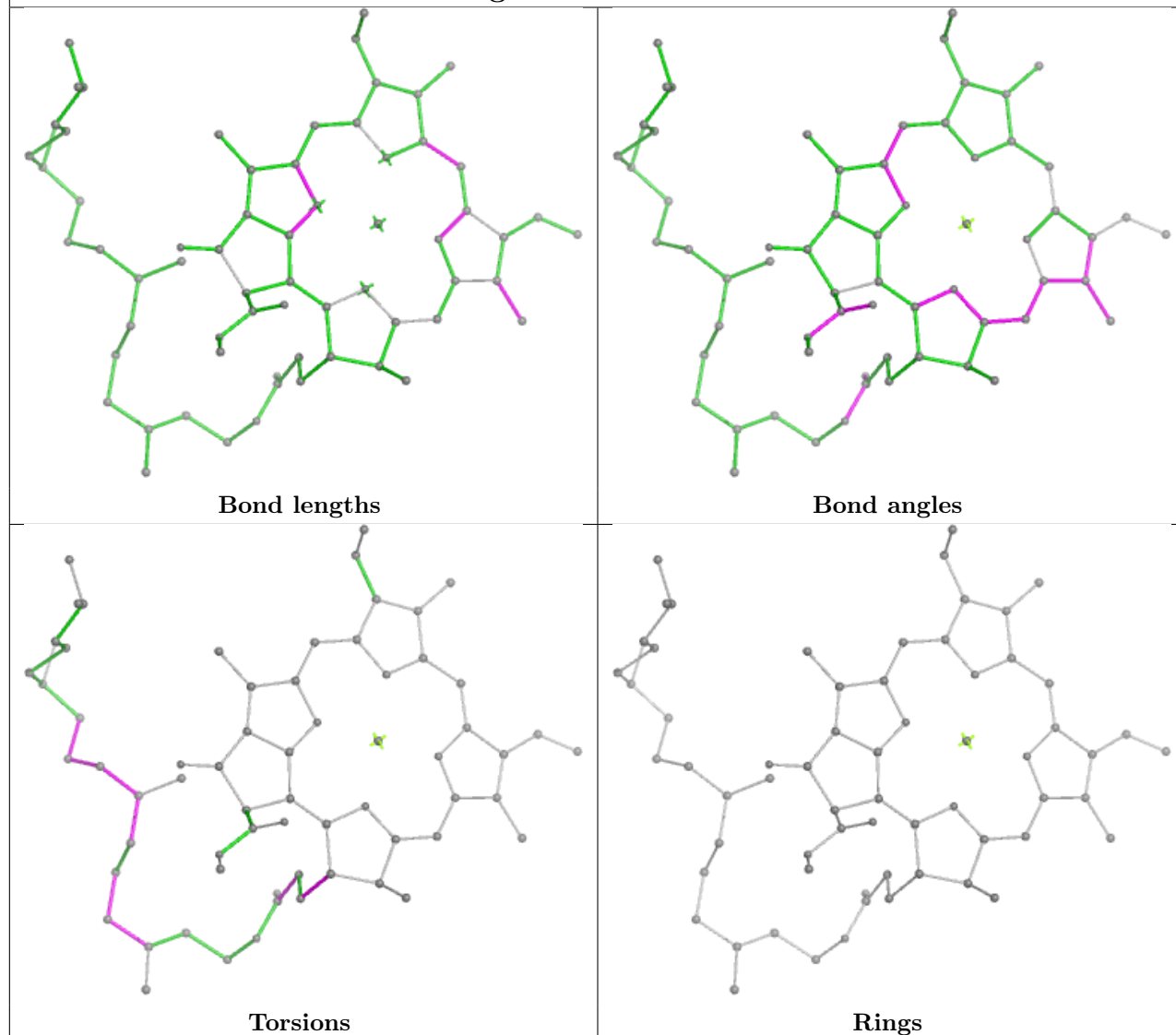
Torsions



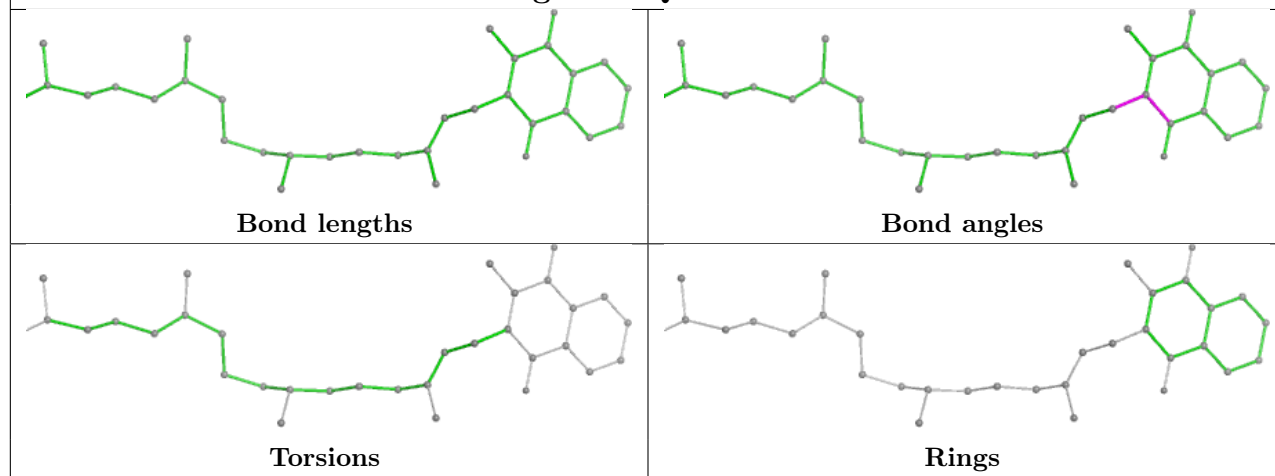
Rings



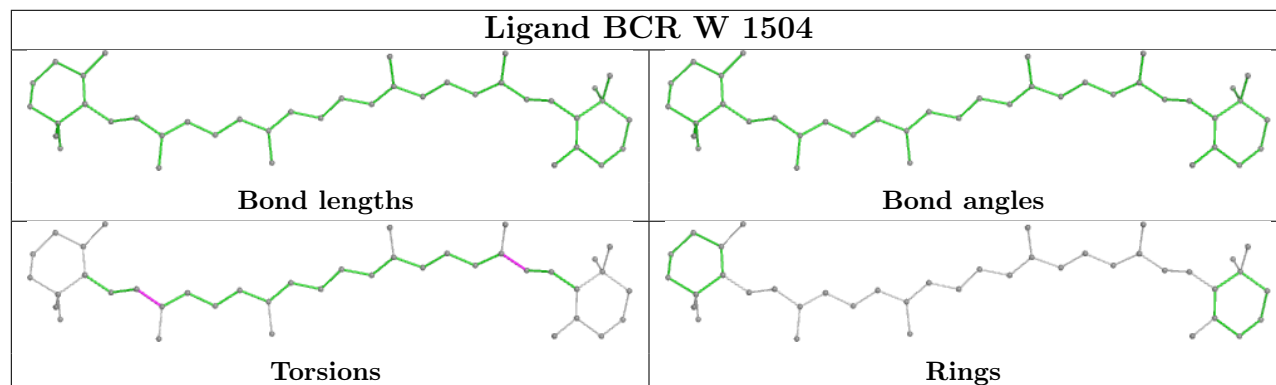
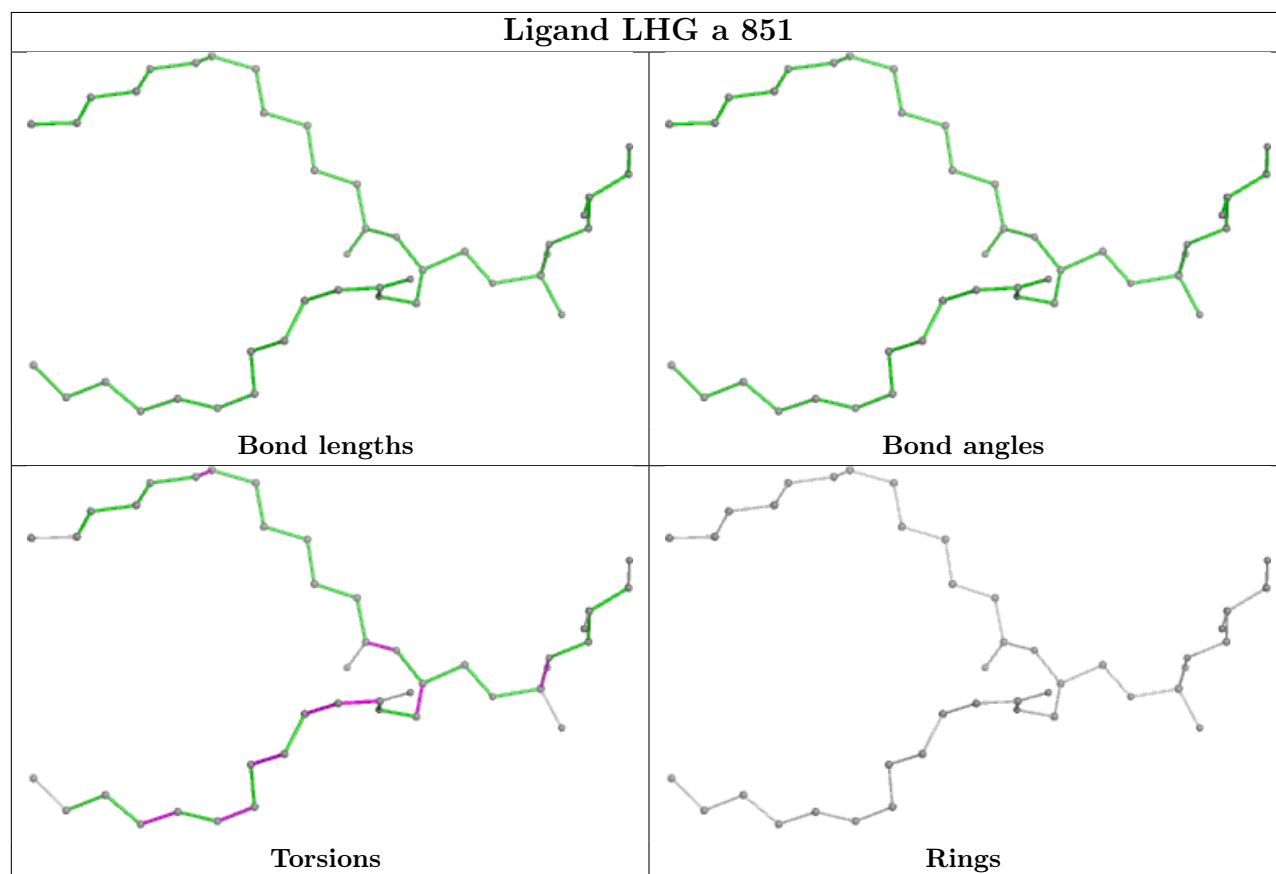
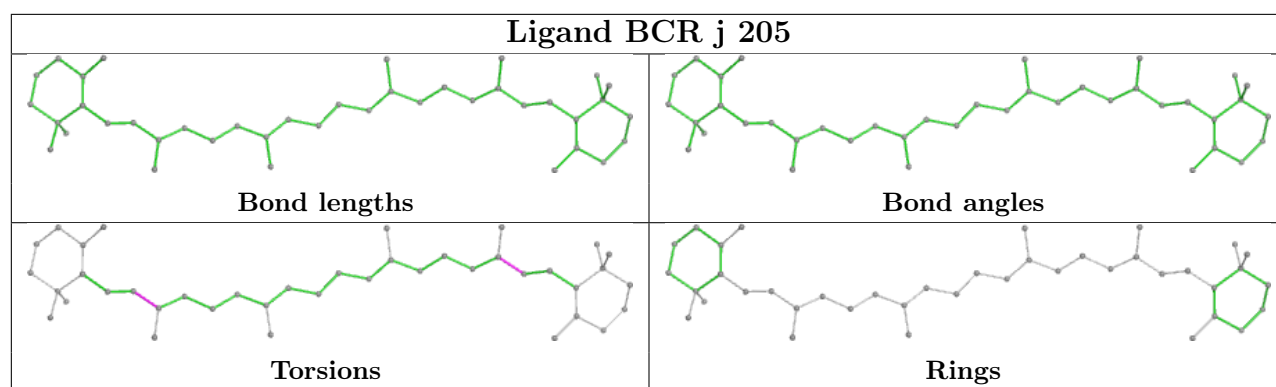
## Ligand CLA O 832



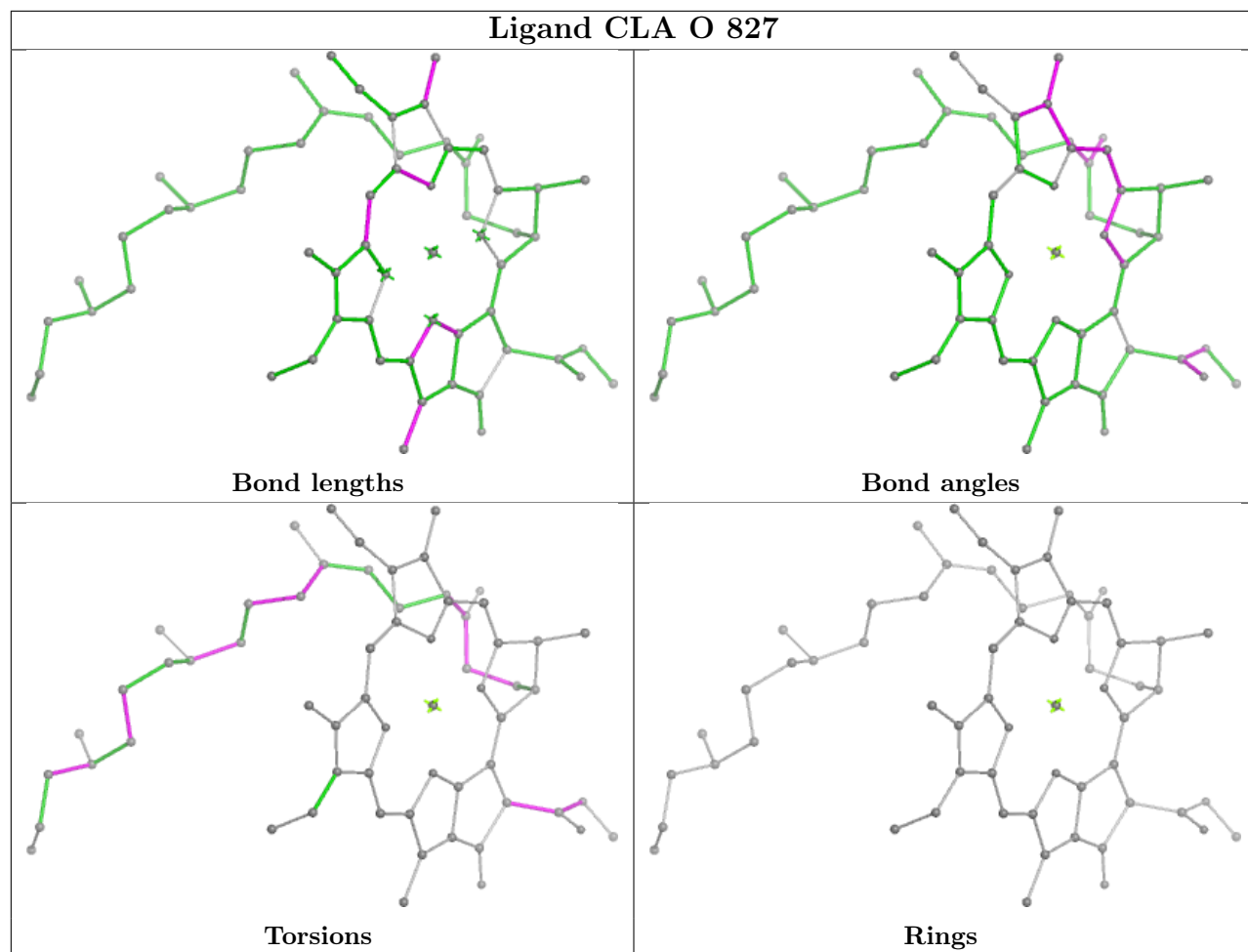
## Ligand PQN a 843





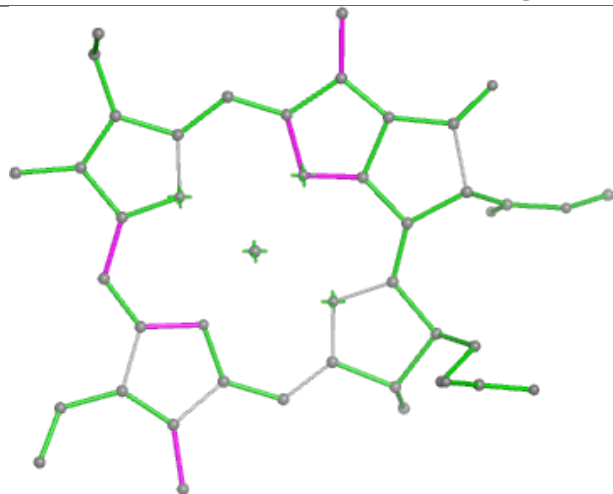




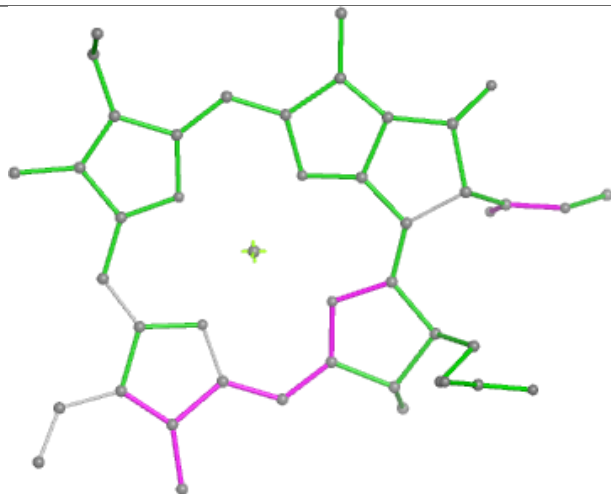




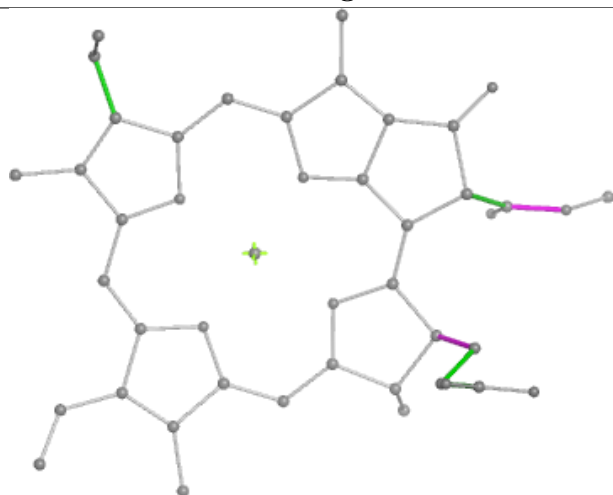
## Ligand CLA b 835



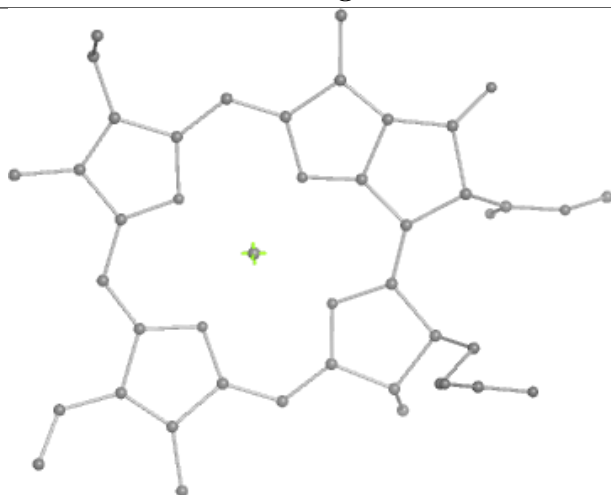
Bond lengths



Bond angles

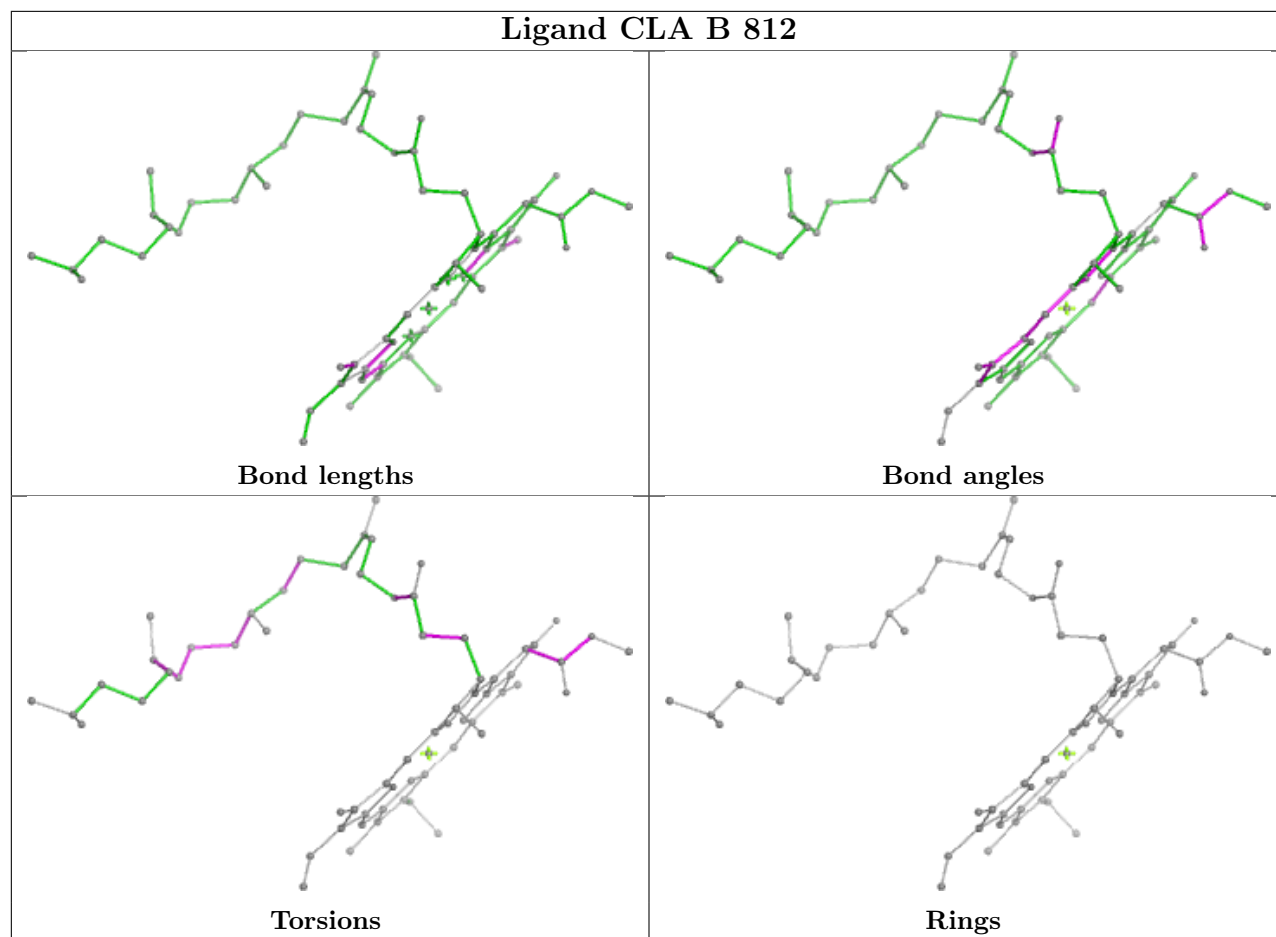
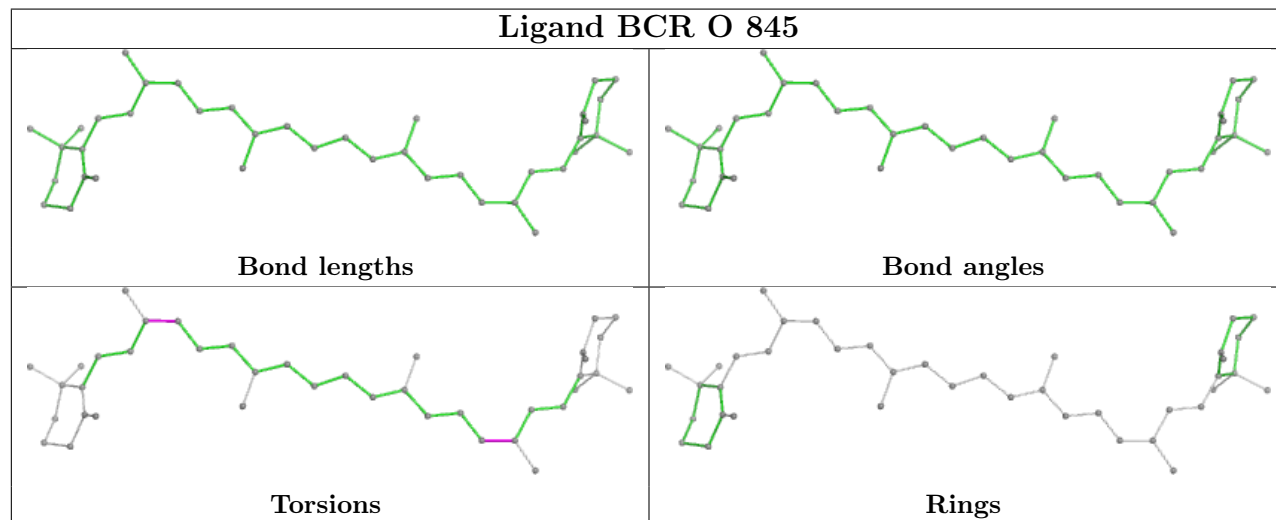


Torsions

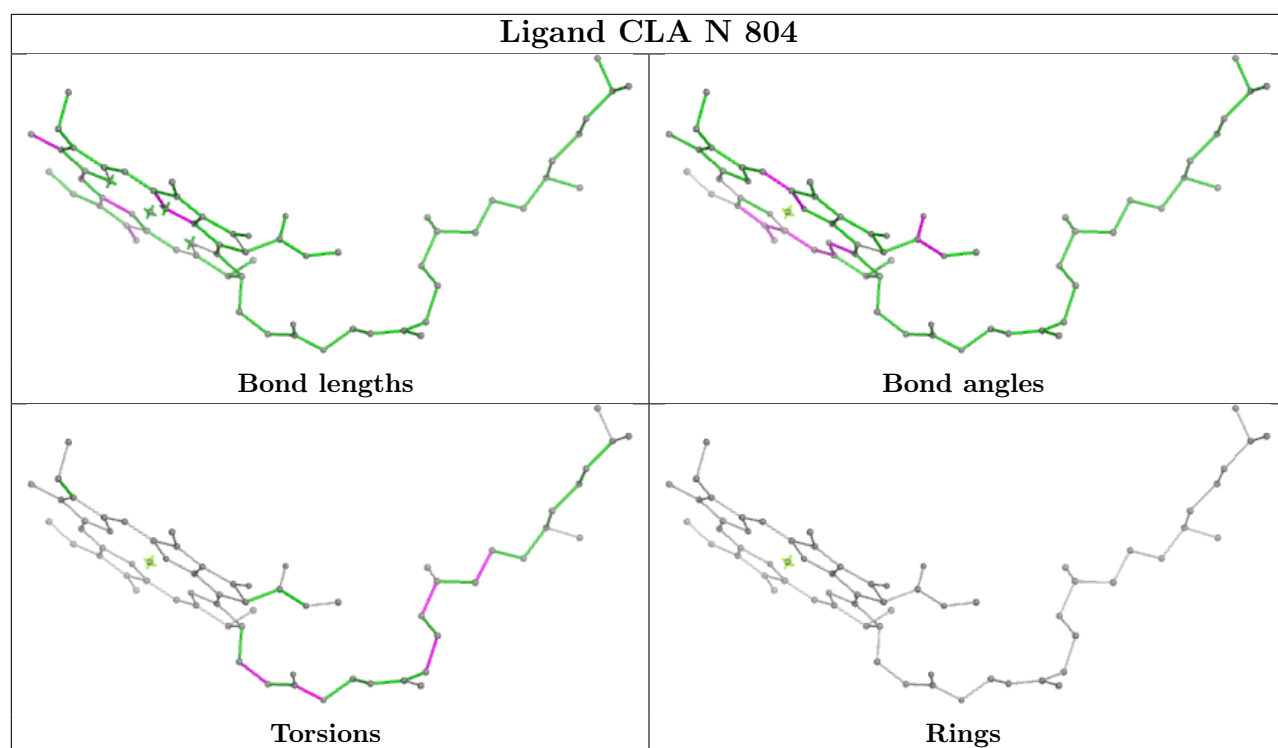


Rings

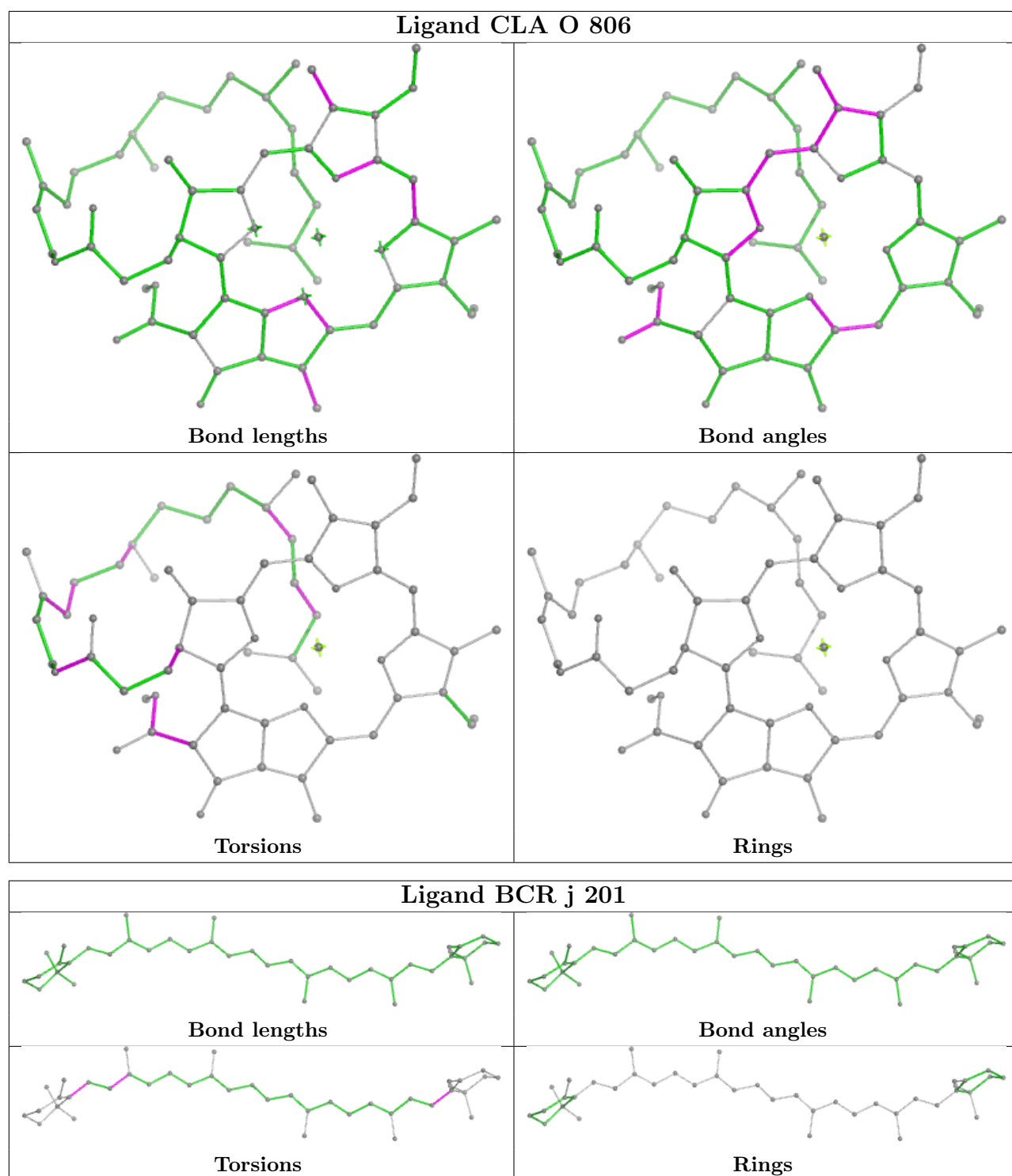


**Ligand CLA B 812****Ligand BCR O 845**

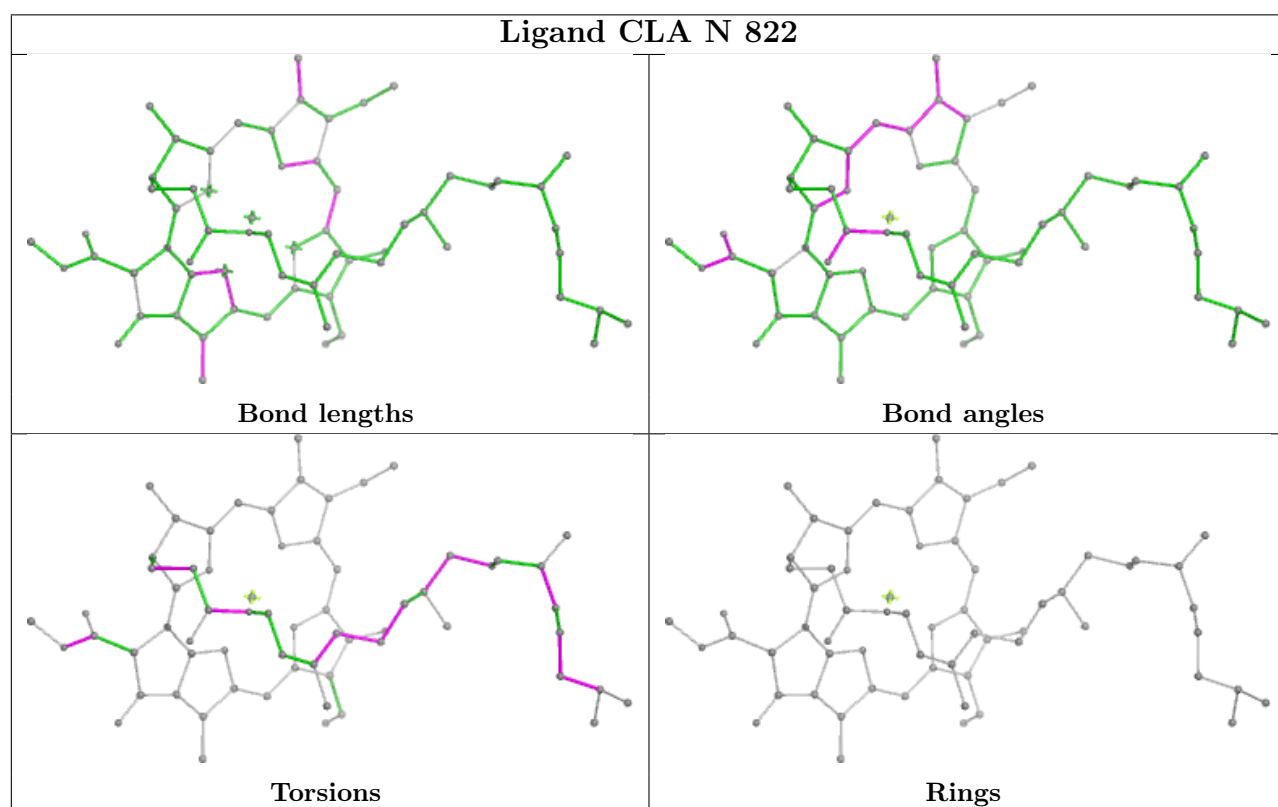
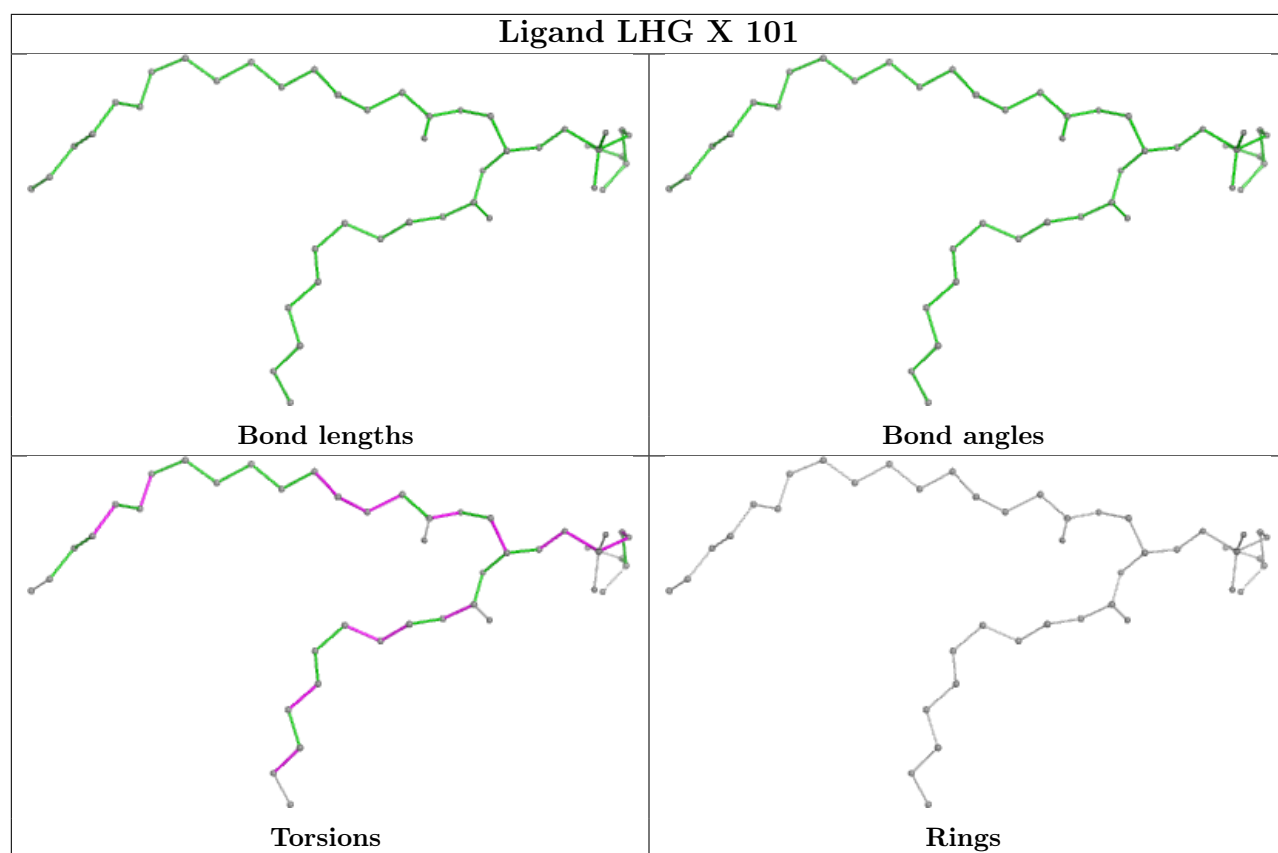






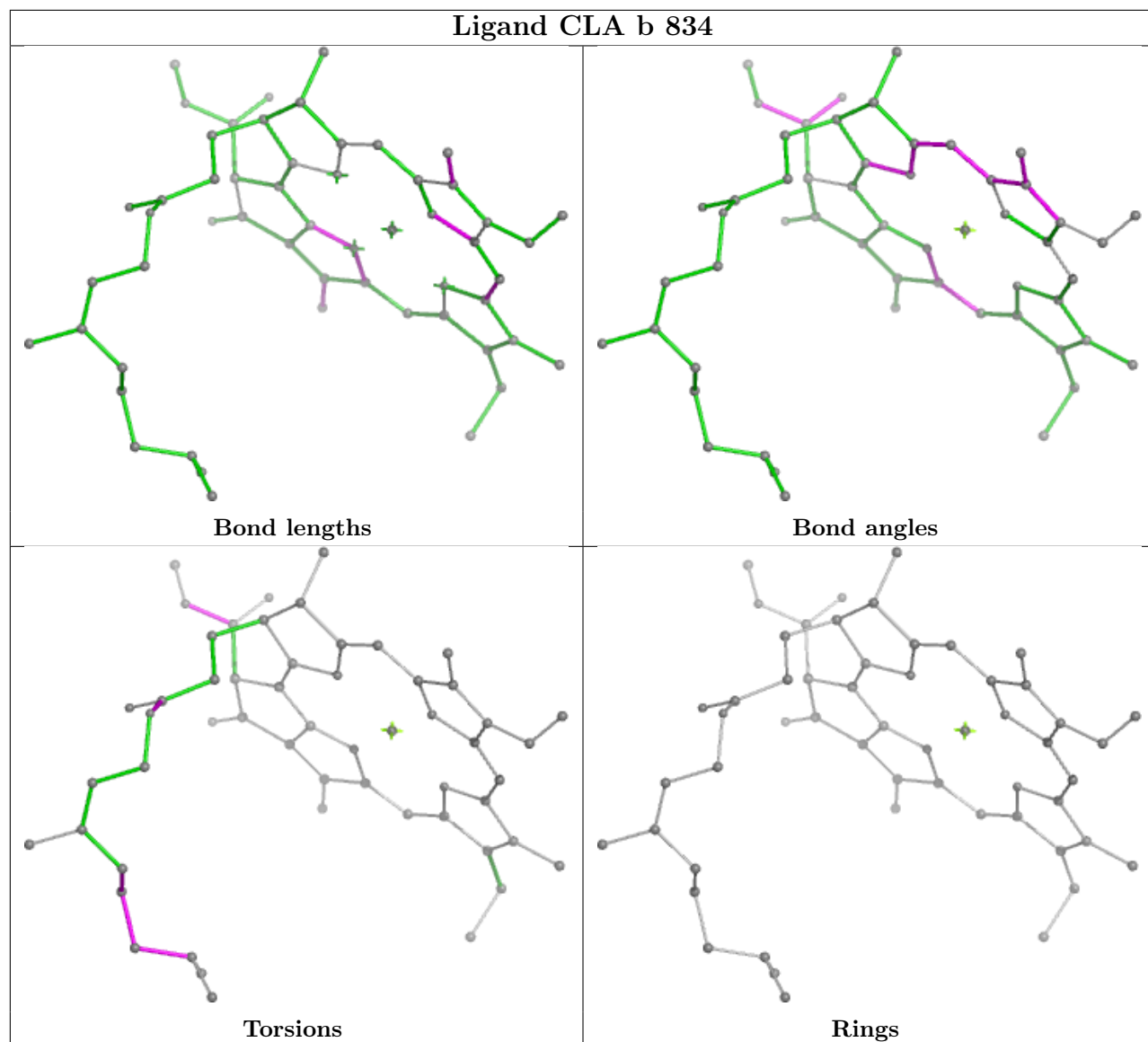




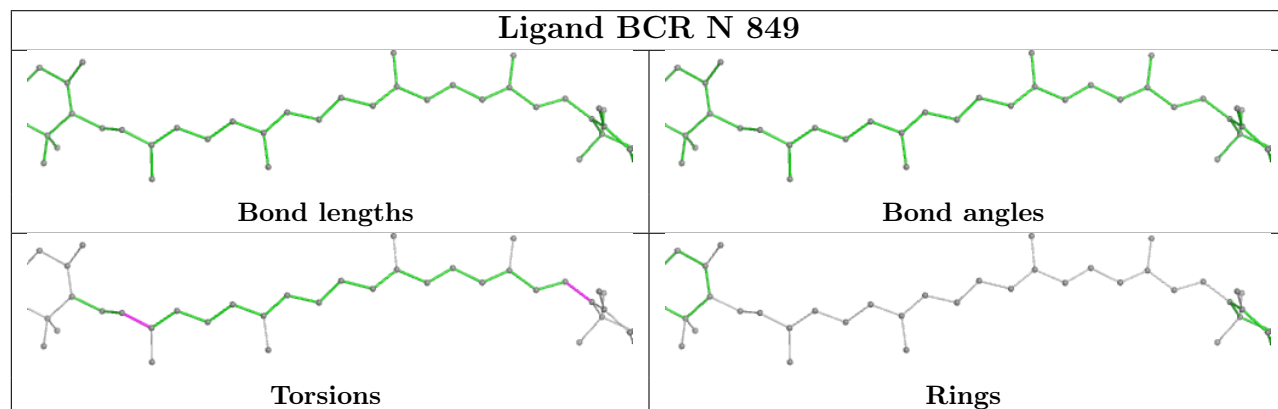




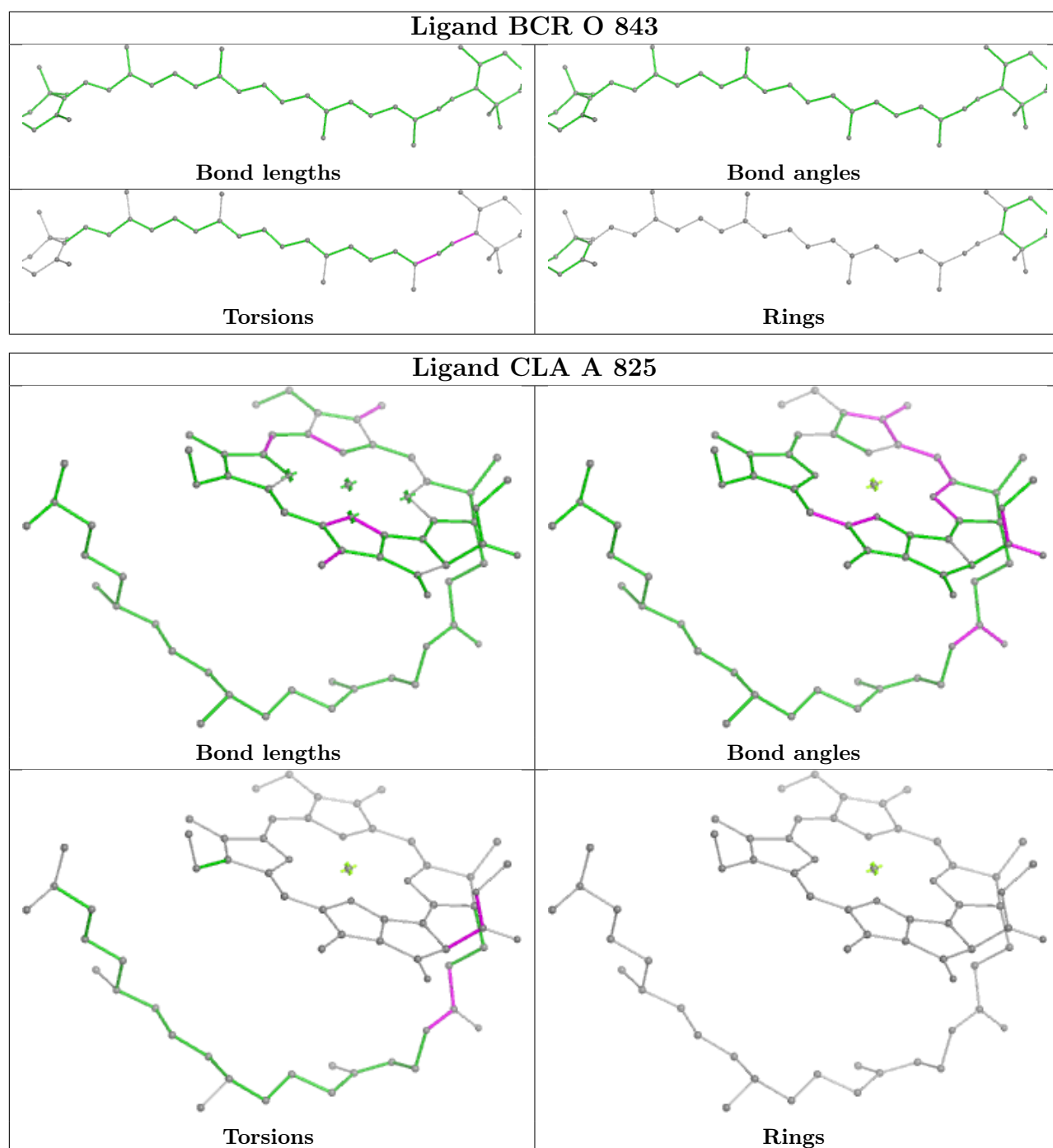
## Ligand CLA b 834



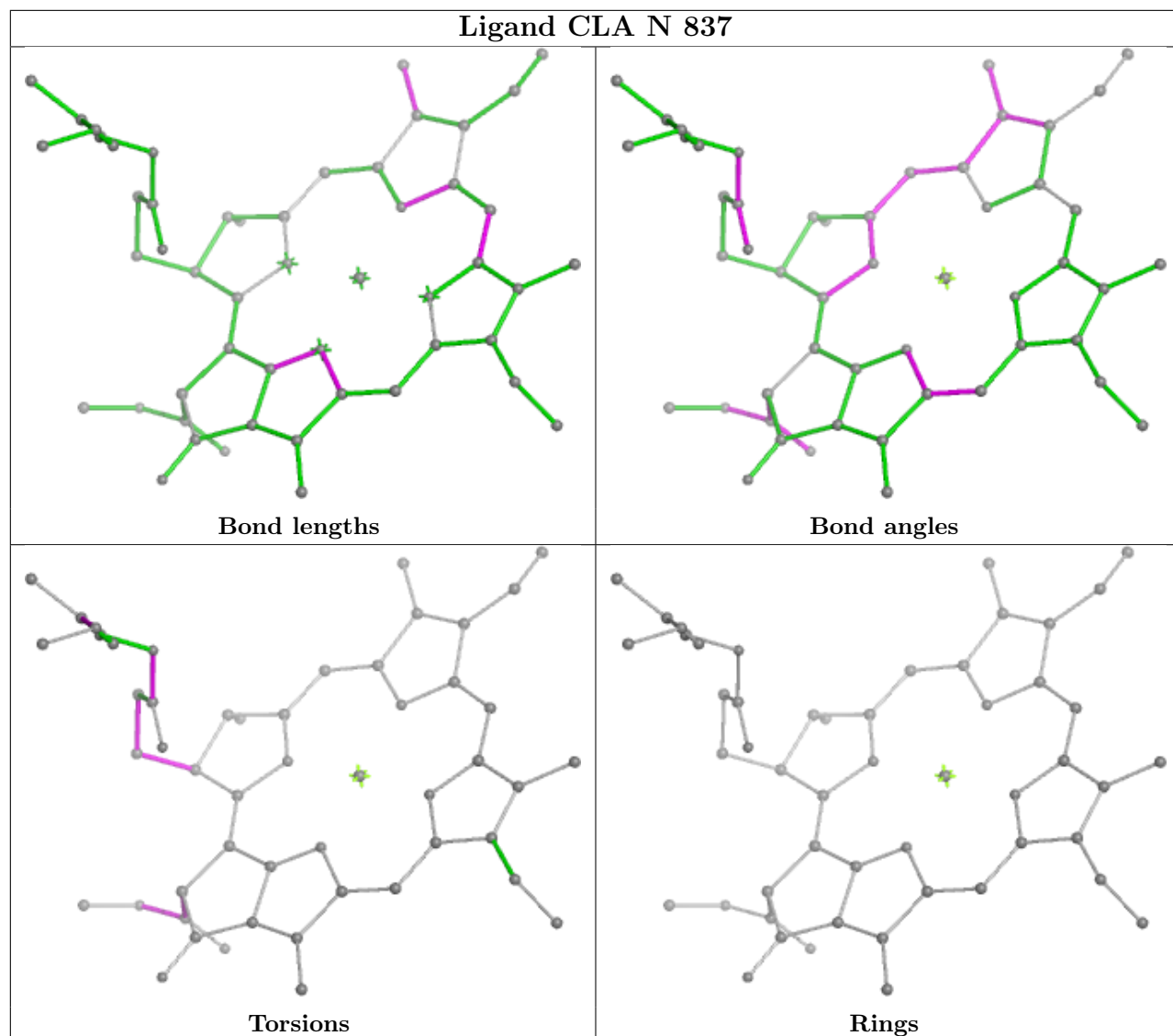
## Ligand BCR N 849



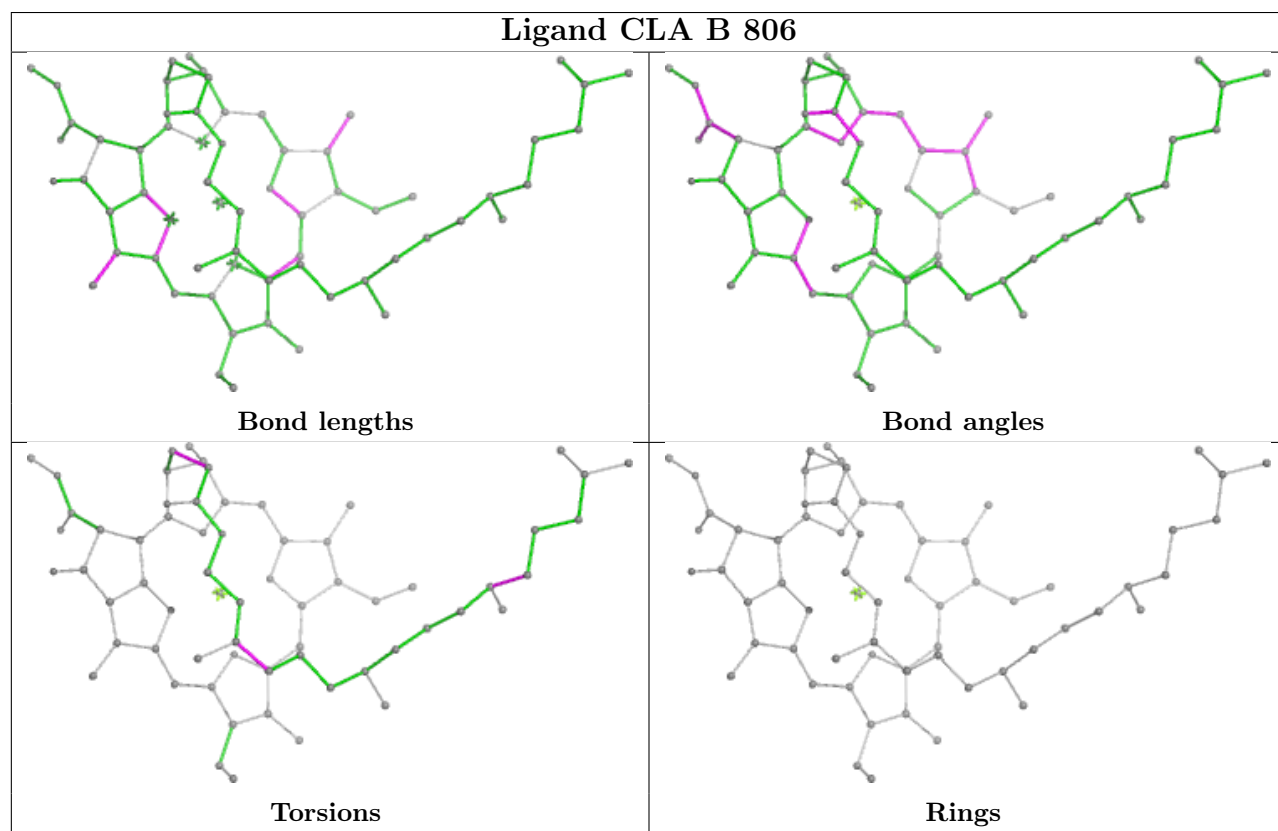
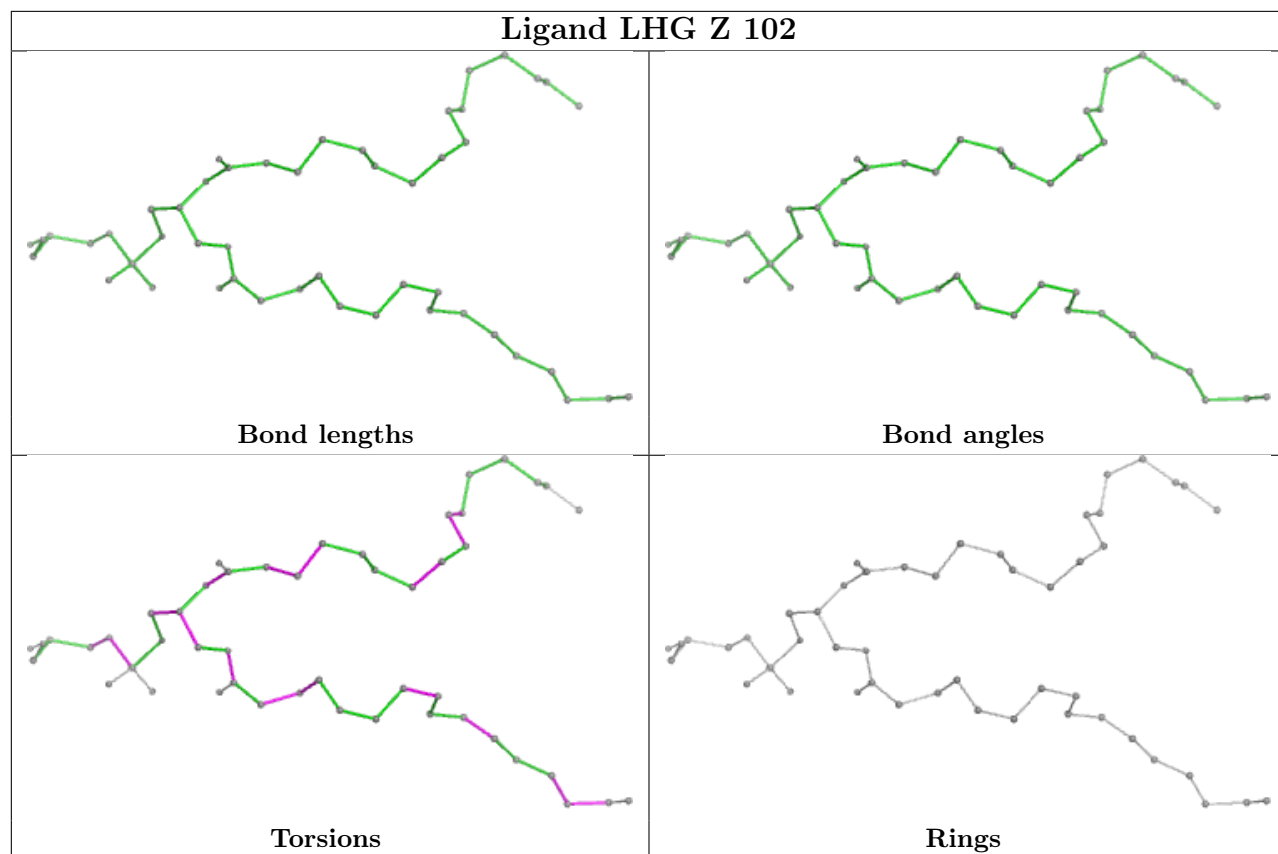




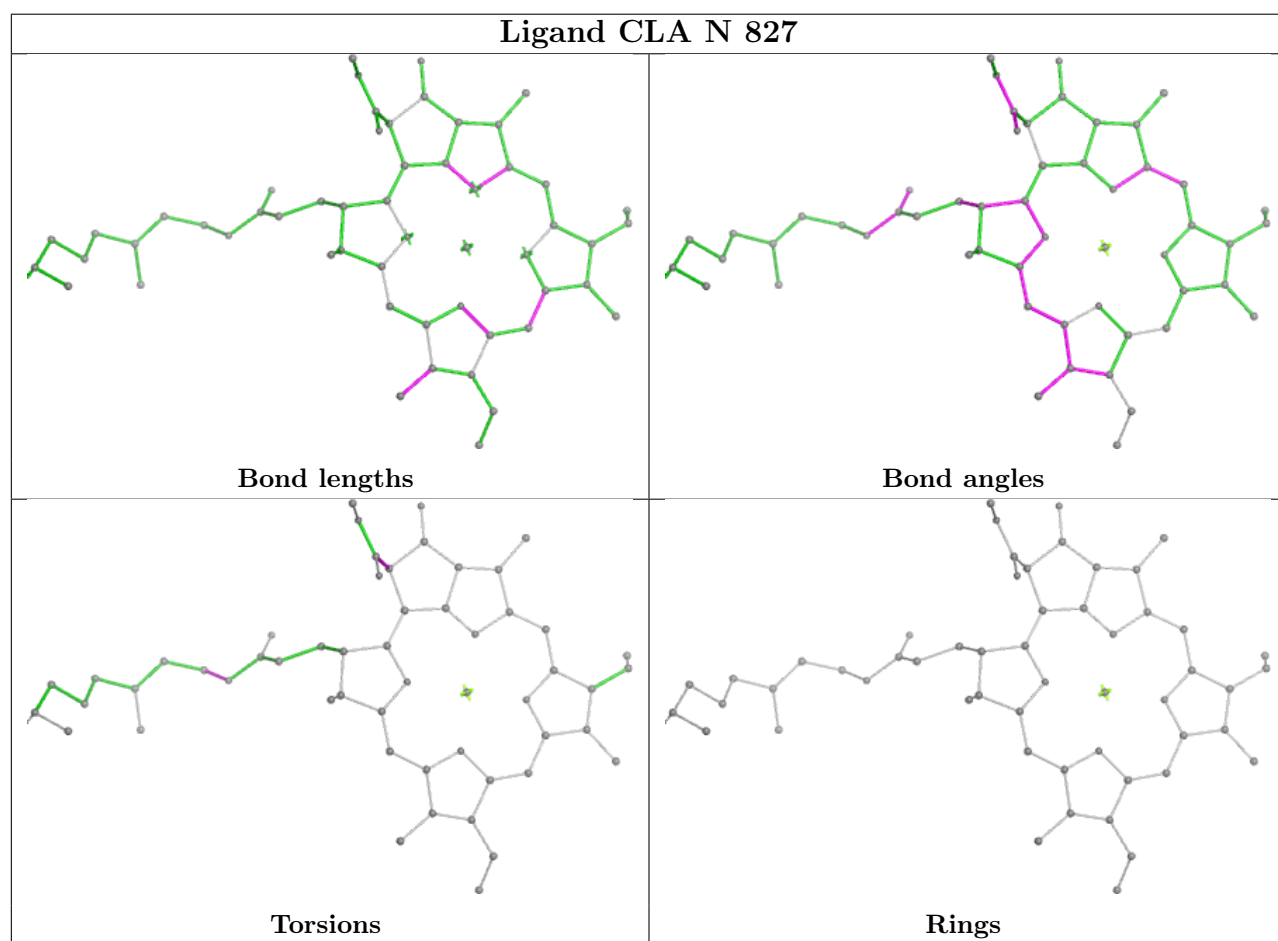
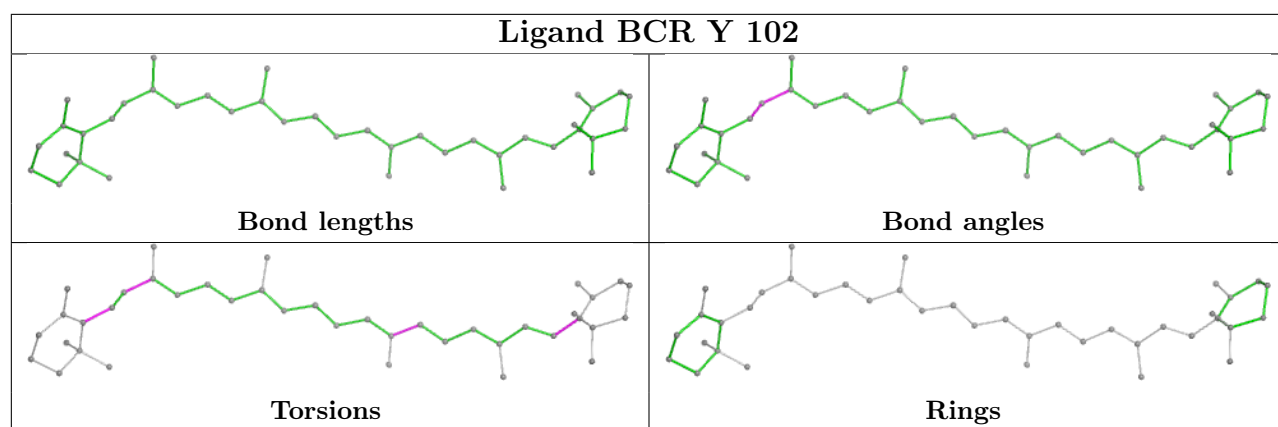






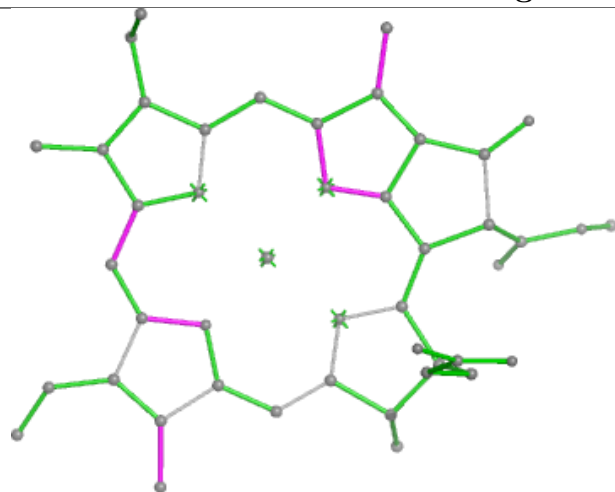




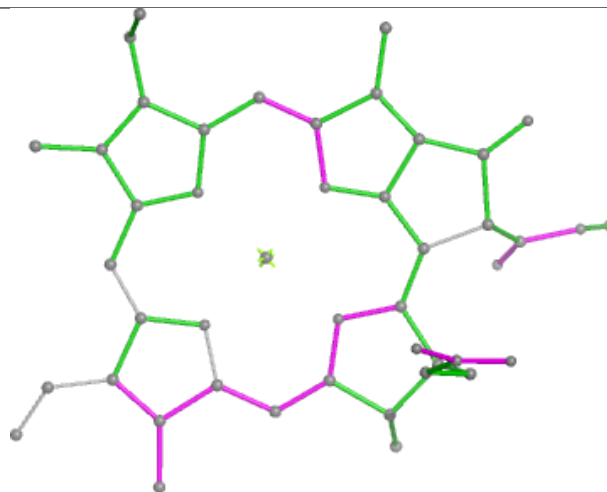




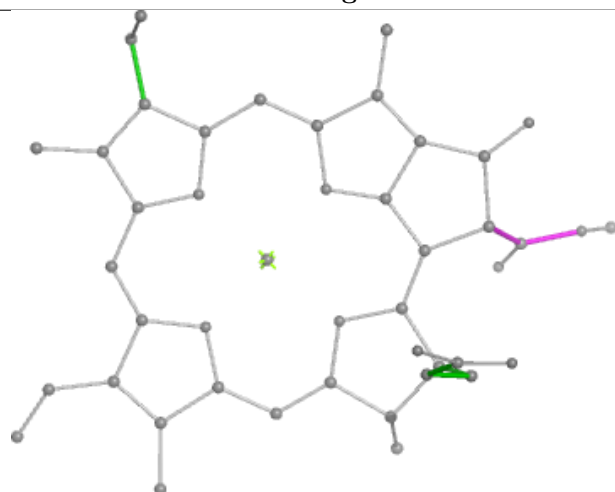
## Ligand CLA N 808



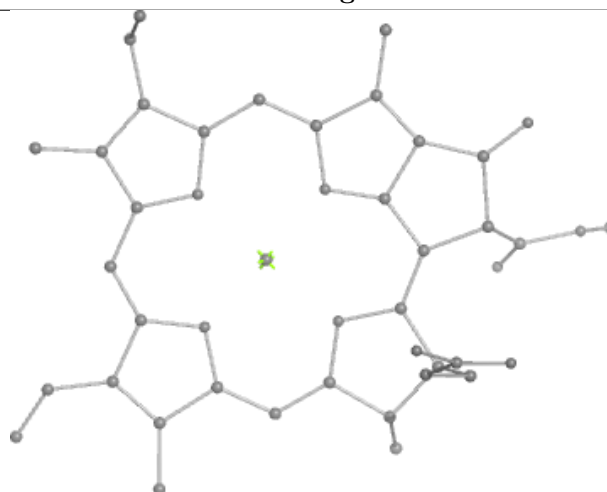
Bond lengths



Bond angles

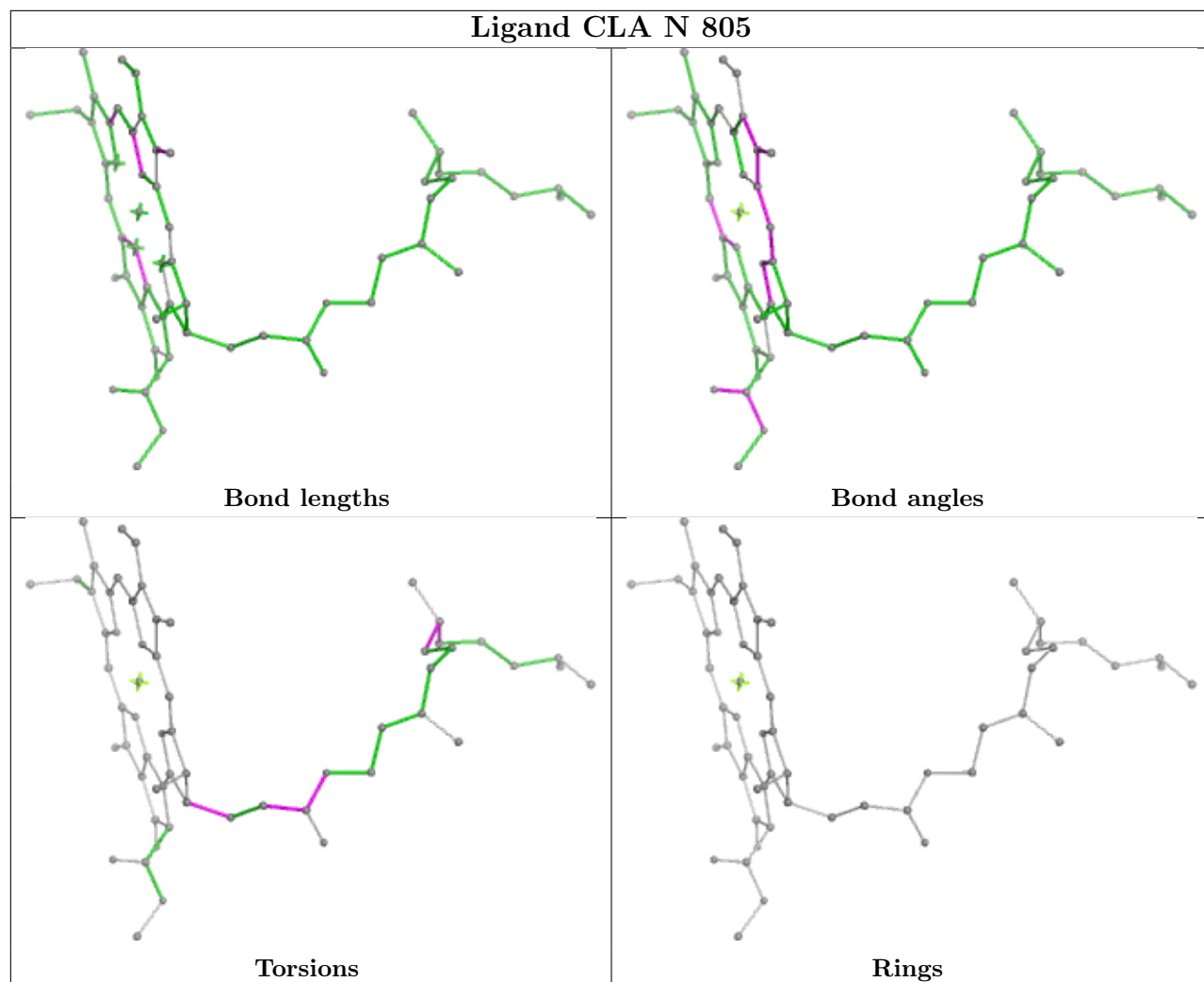


Torsions

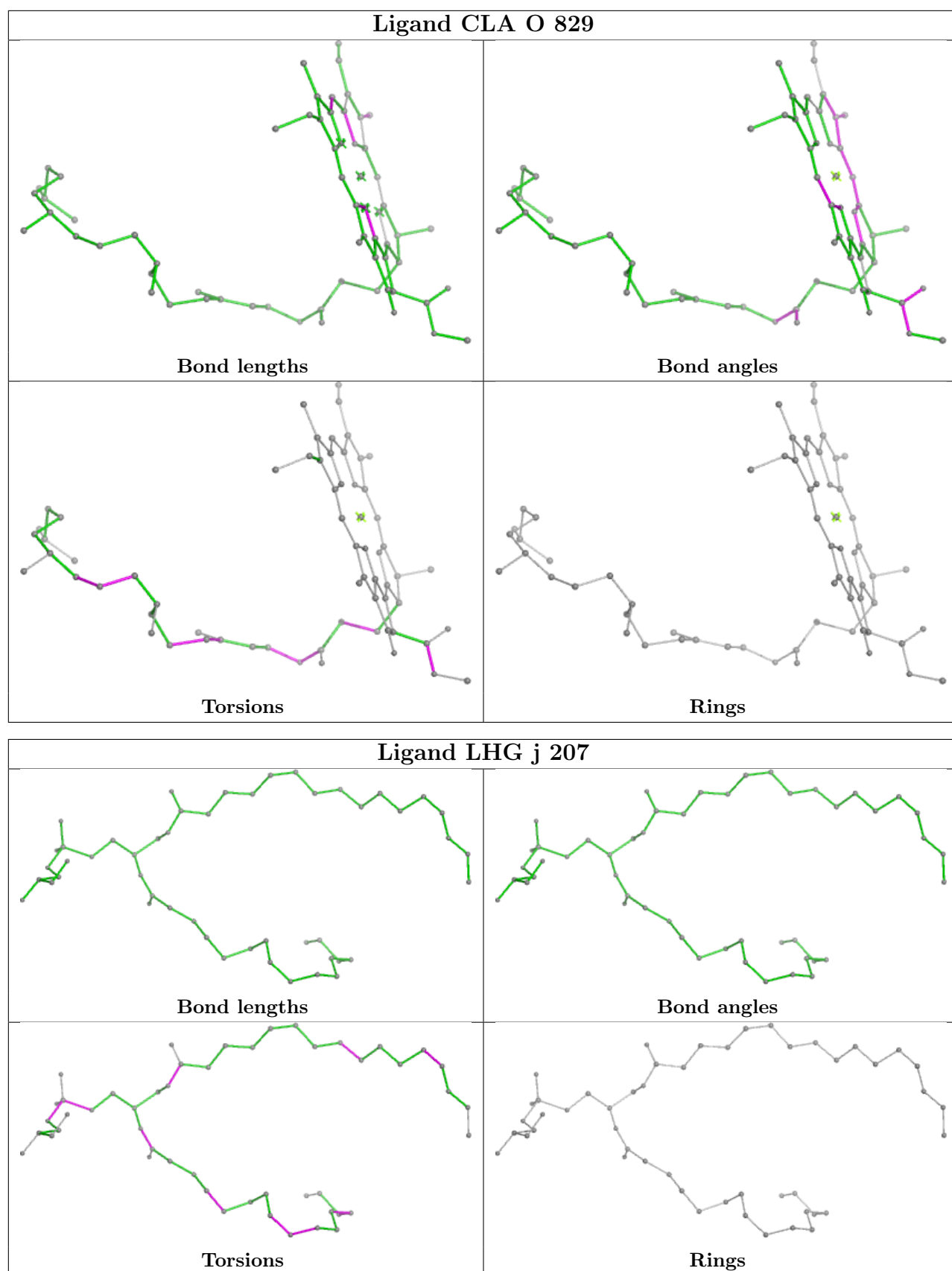


Rings

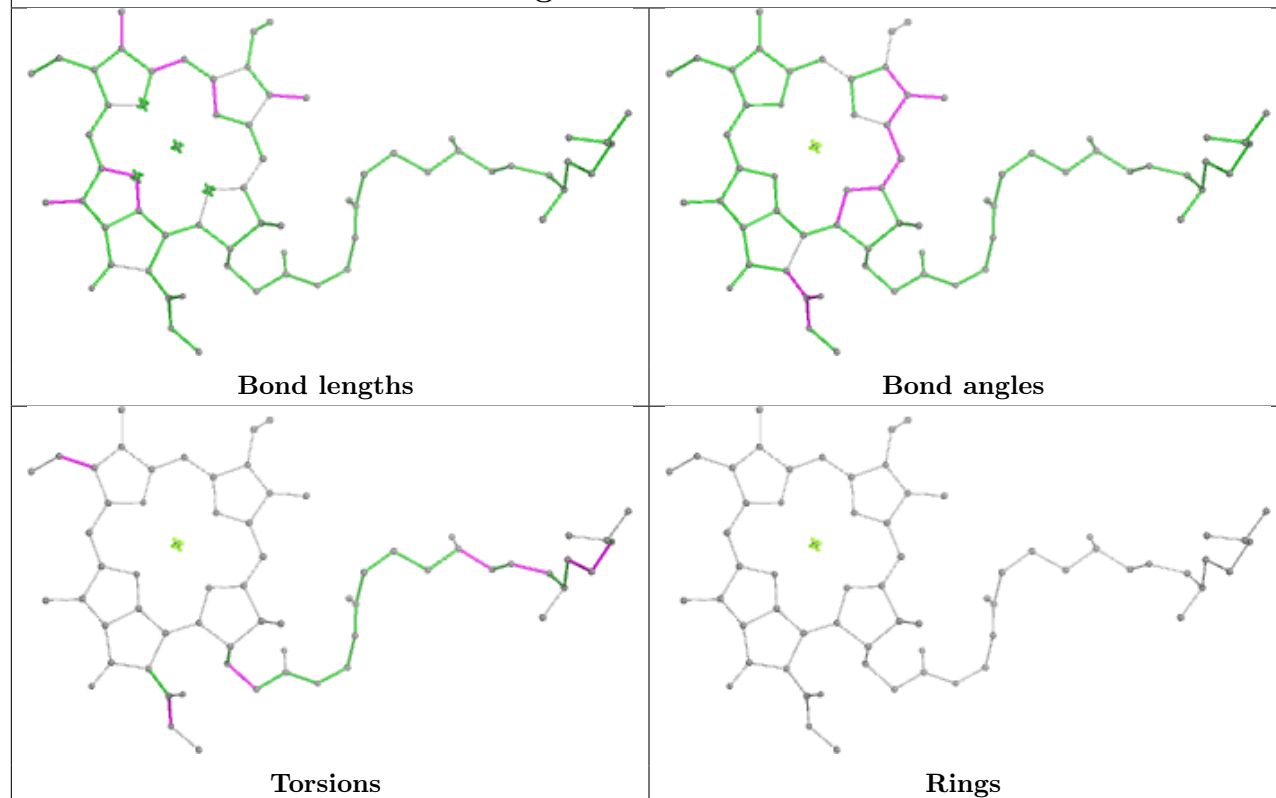
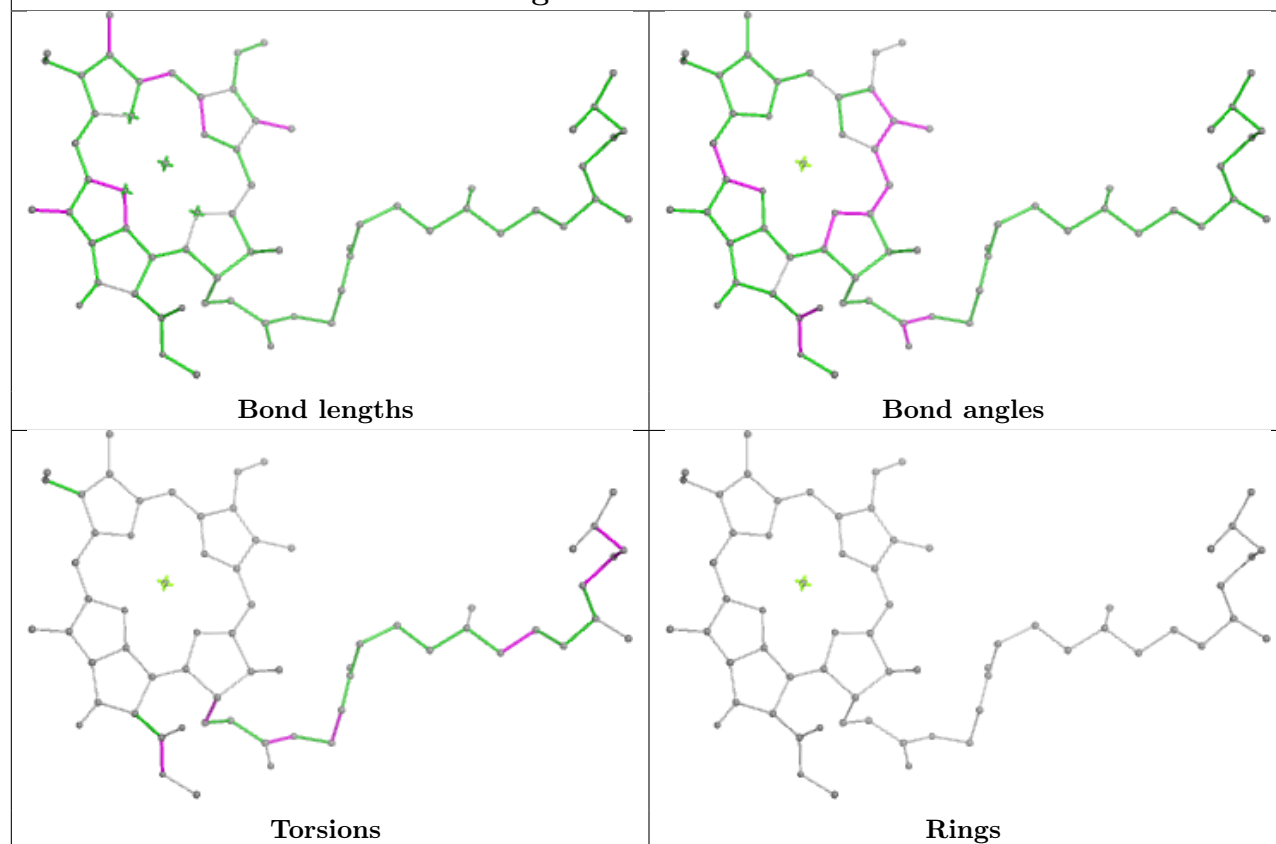




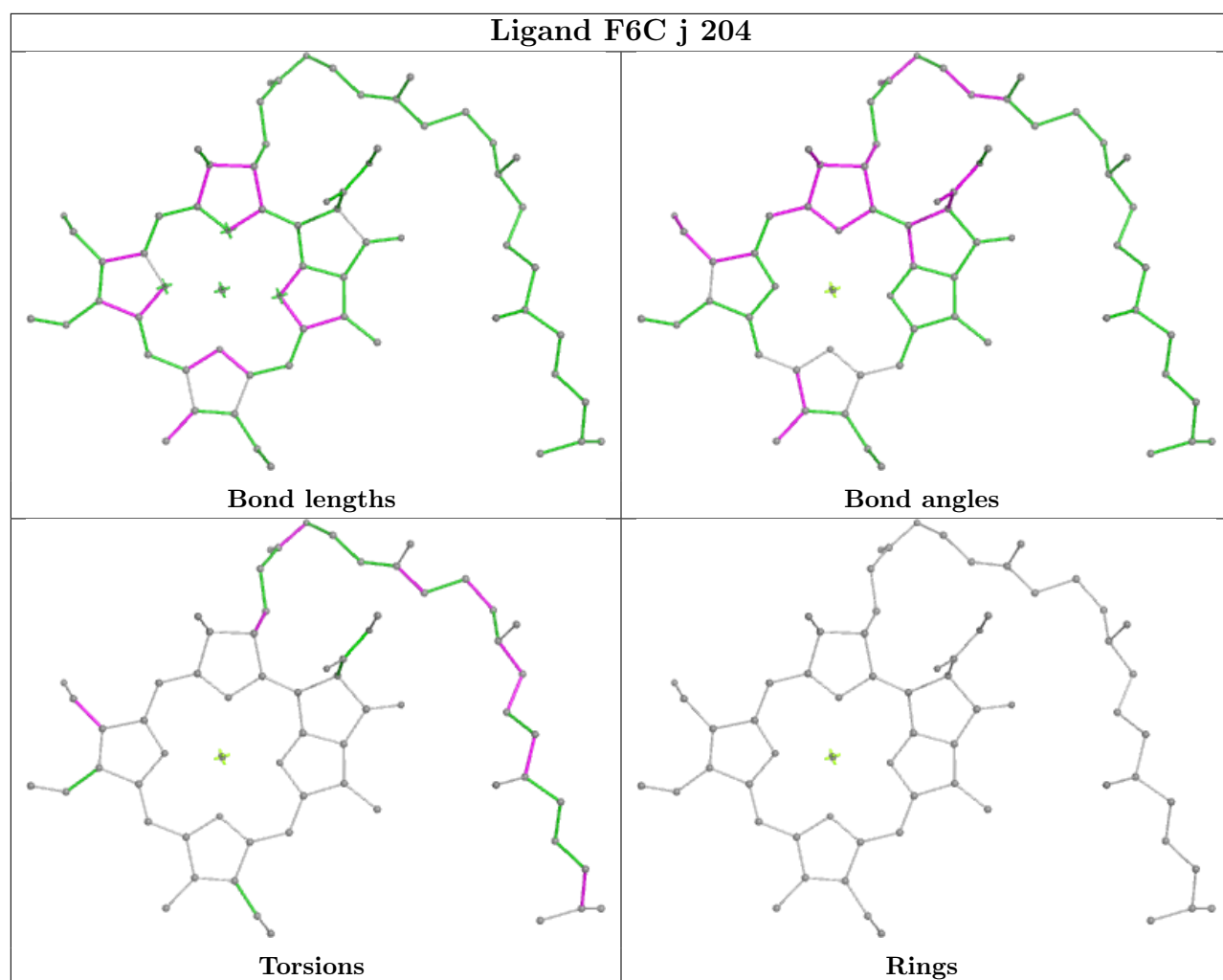






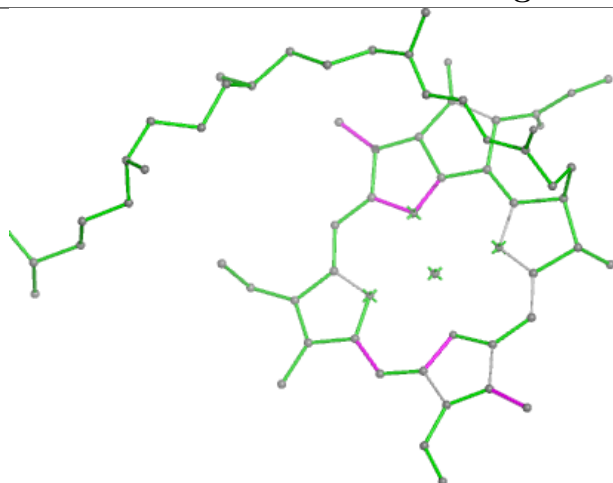
**Ligand CLA b 803****Ligand CLA A 803**



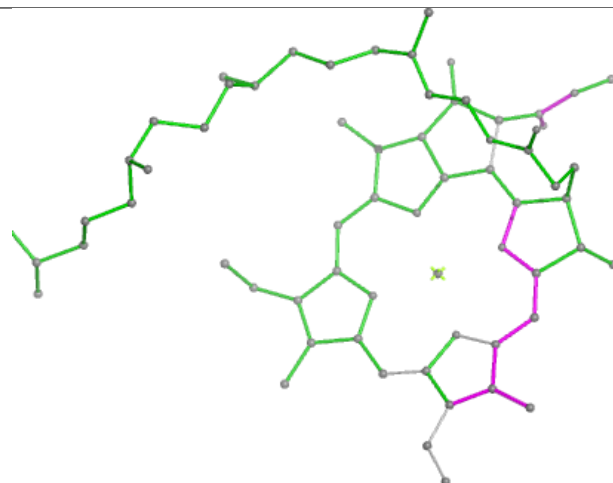




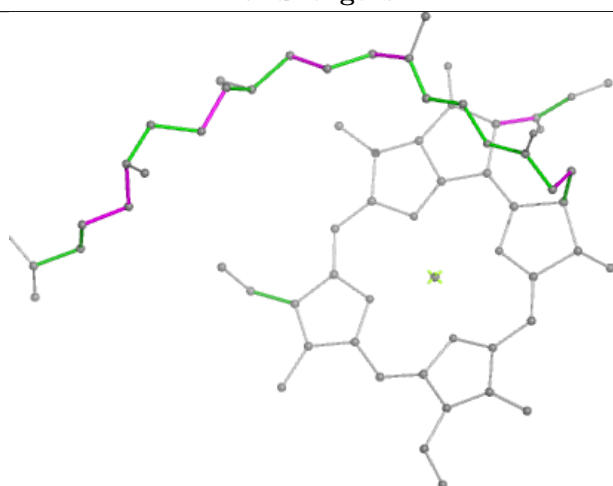
## Ligand CLA A 830



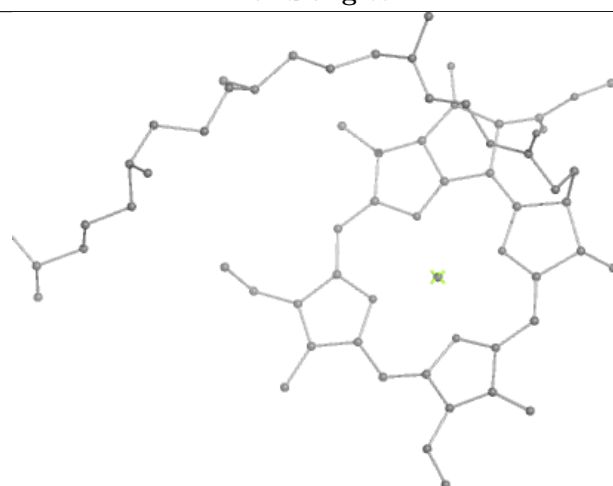
Bond lengths



Bond angles

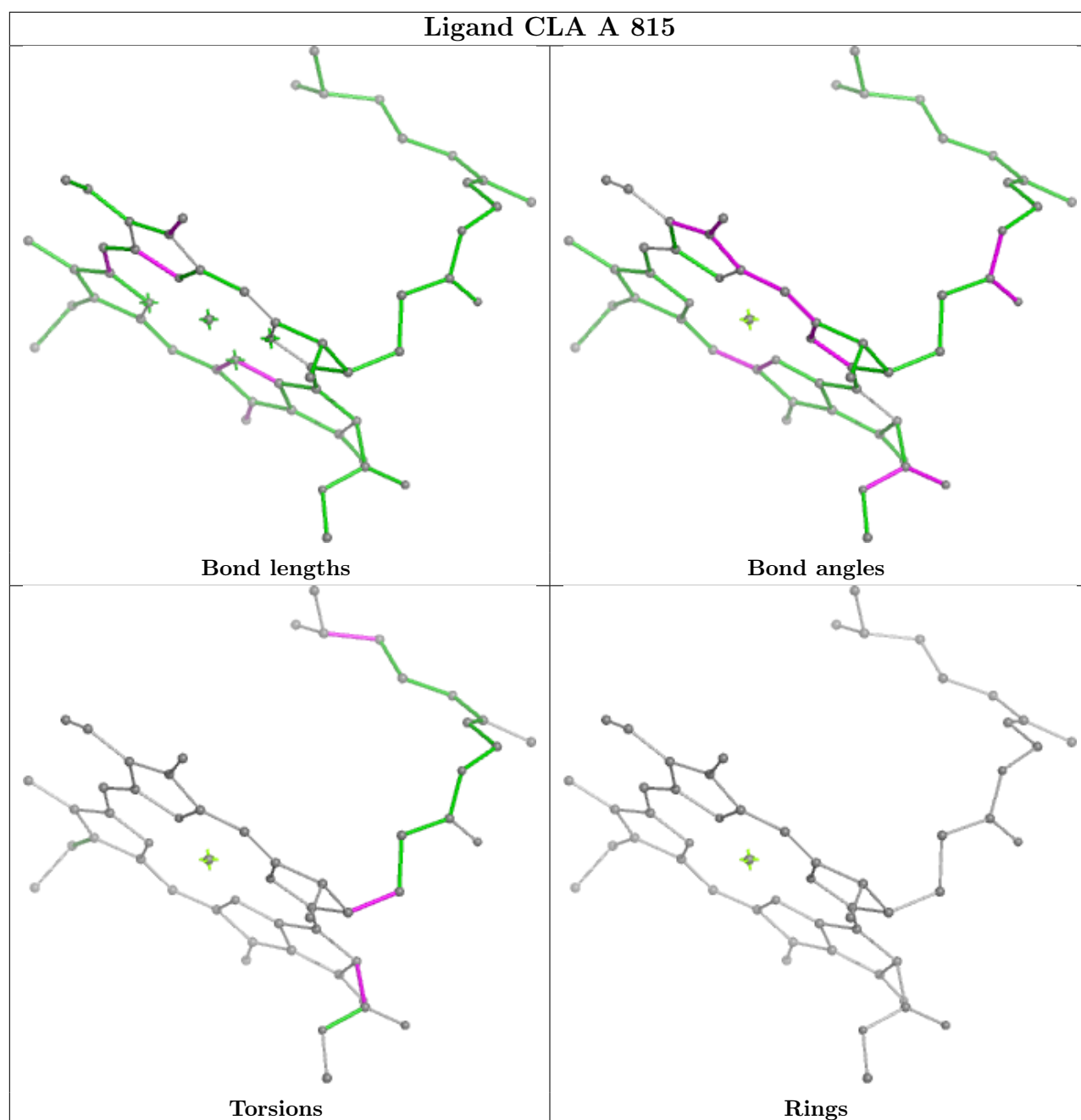


Torsions



Rings





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



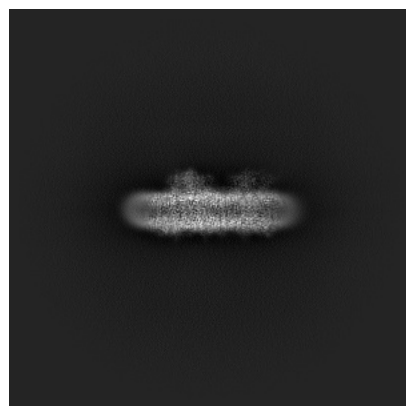
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50063. These allow visual inspection of the internal detail of the map and identification of artifacts.

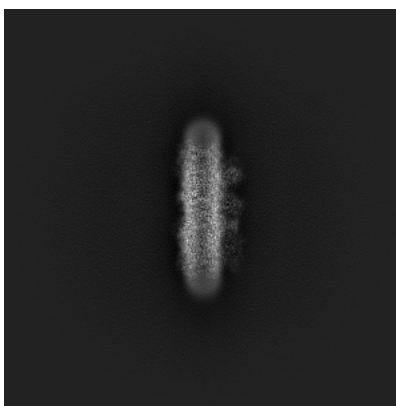
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

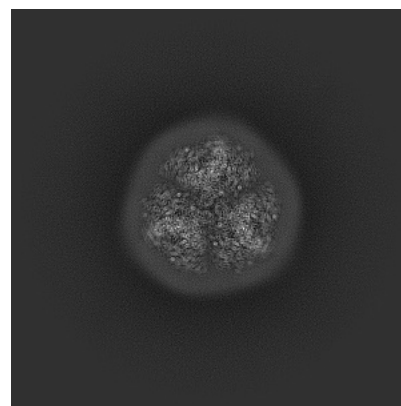
#### 6.1.1 Primary map



X

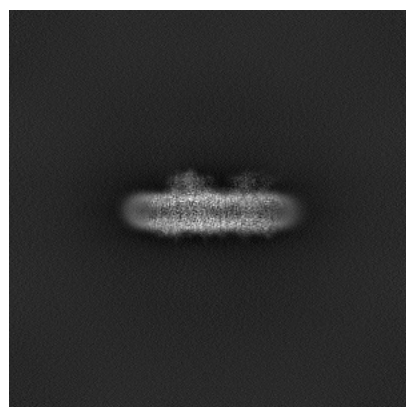


Y

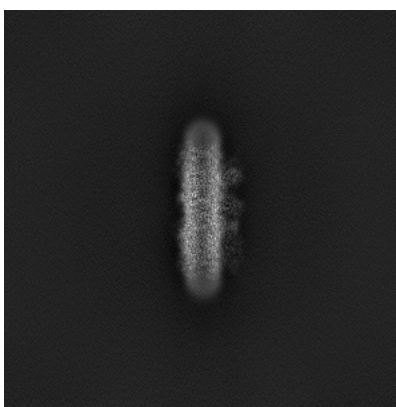


Z

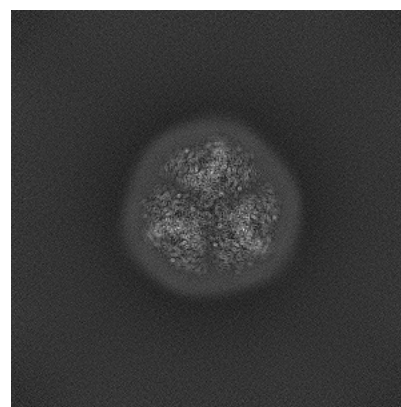
#### 6.1.2 Raw map



X



Y



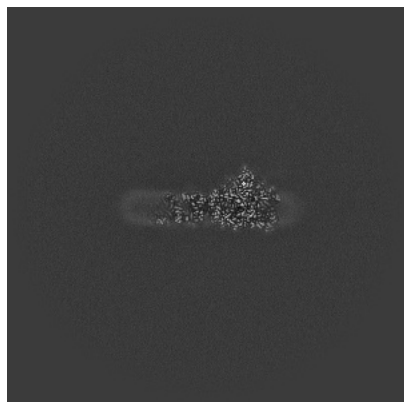
Z

The images above show the map projected in three orthogonal directions.

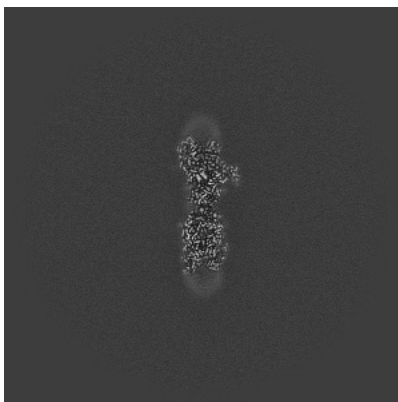


## 6.2 Central slices [i](#)

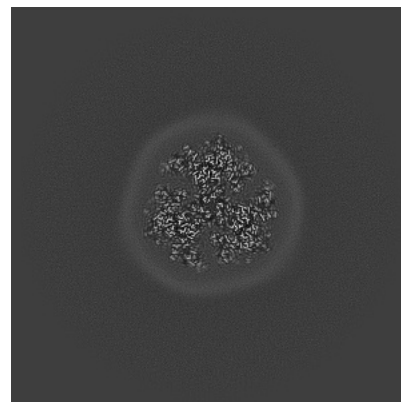
### 6.2.1 Primary map



X Index: 300

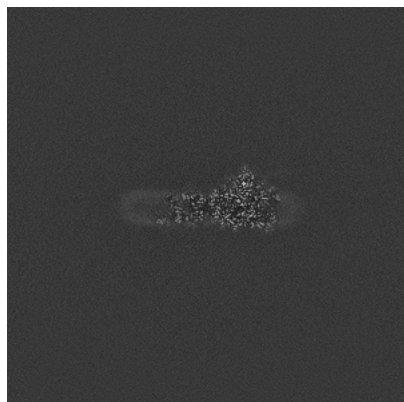


Y Index: 300

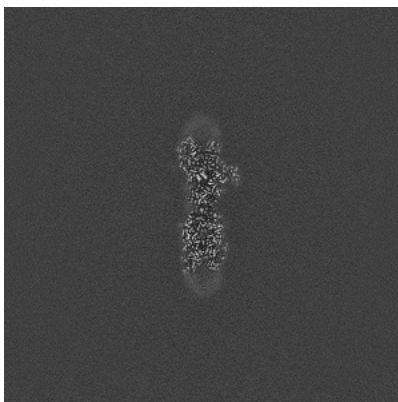


Z Index: 300

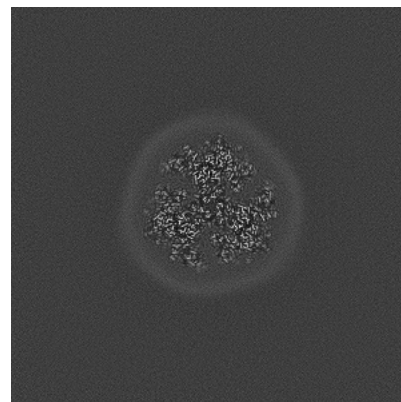
### 6.2.2 Raw map



X Index: 300



Y Index: 300



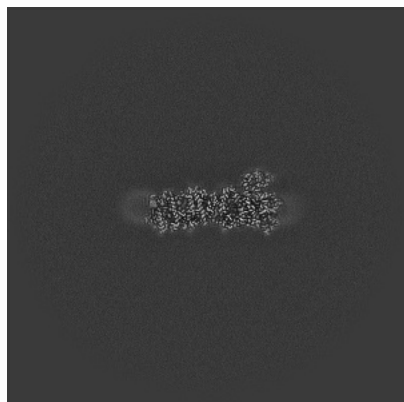
Z Index: 300

The images above show central slices of the map in three orthogonal directions.

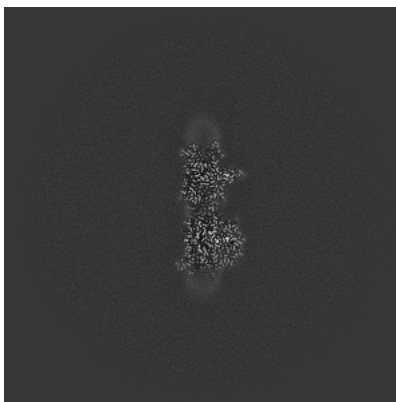


## 6.3 Largest variance slices [i](#)

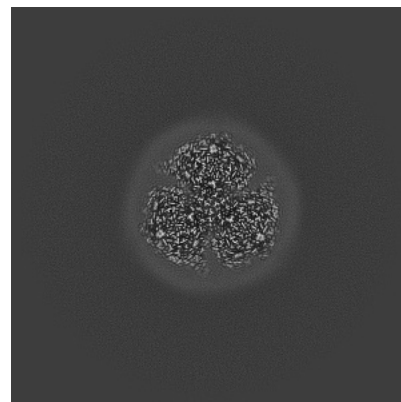
### 6.3.1 Primary map



X Index: 314

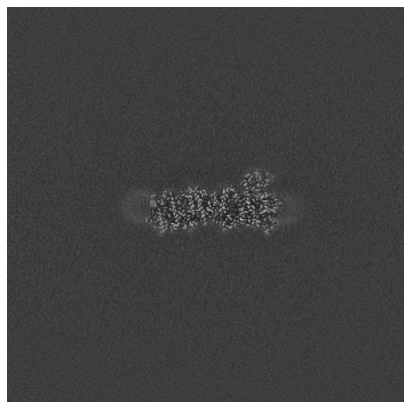


Y Index: 273

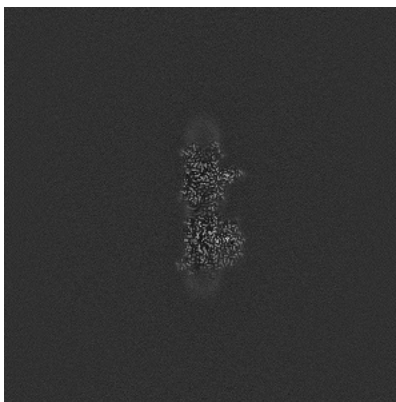


Z Index: 312

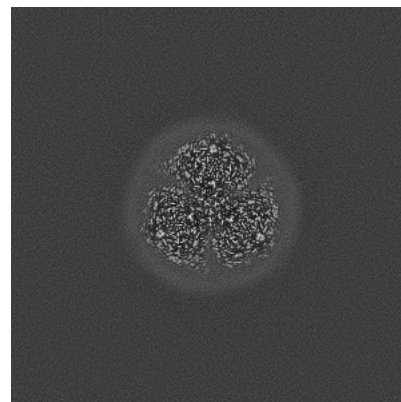
### 6.3.2 Raw map



X Index: 314



Y Index: 273



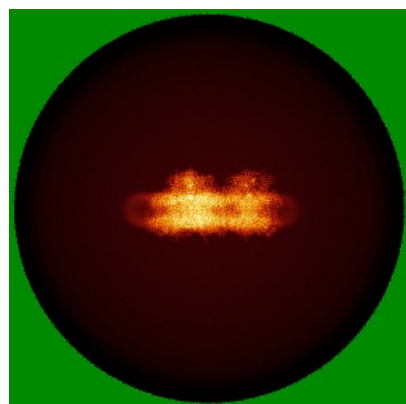
Z Index: 312

The images above show the largest variance slices of the map in three orthogonal directions.

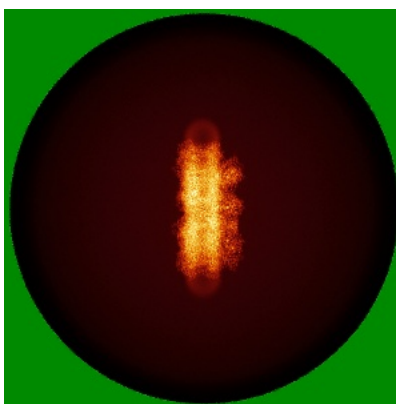


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

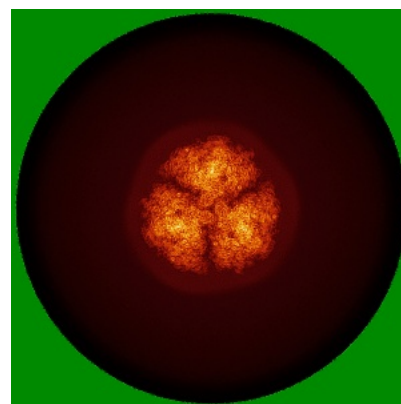
### 6.4.1 Primary map



X

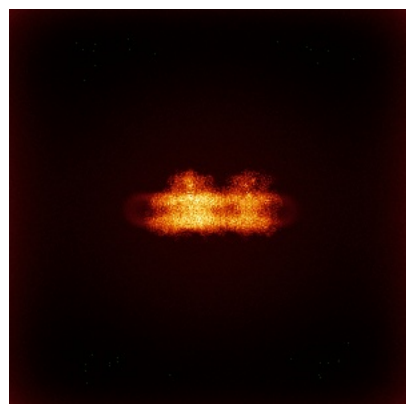


Y

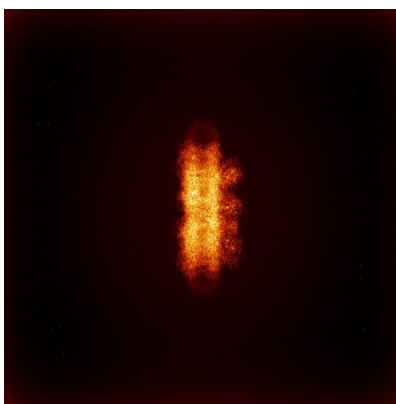


Z

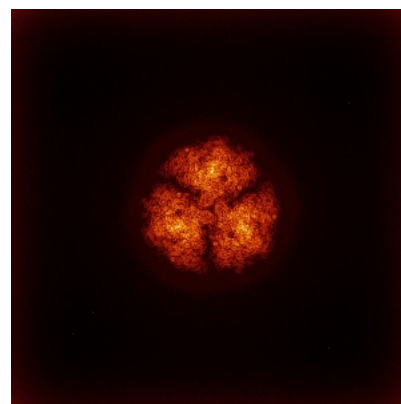
### 6.4.2 Raw map



X



Y



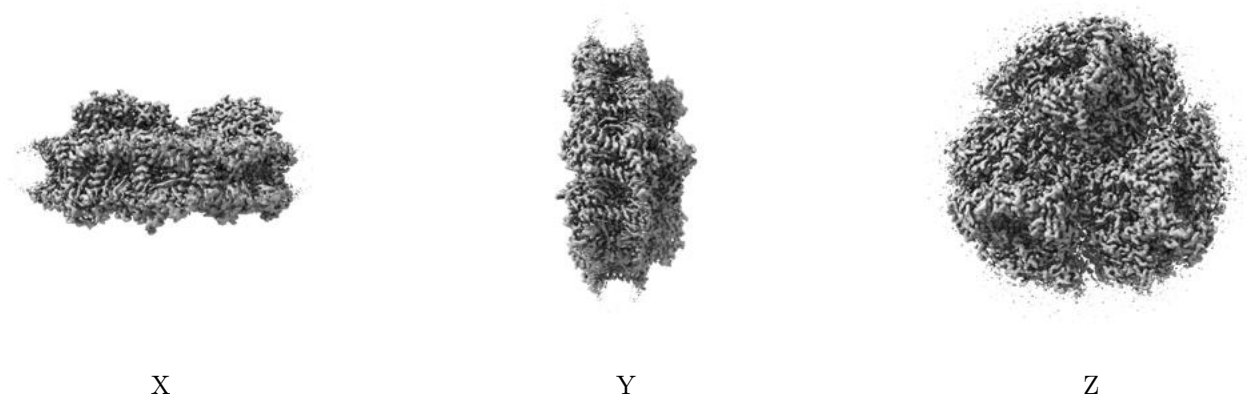
Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



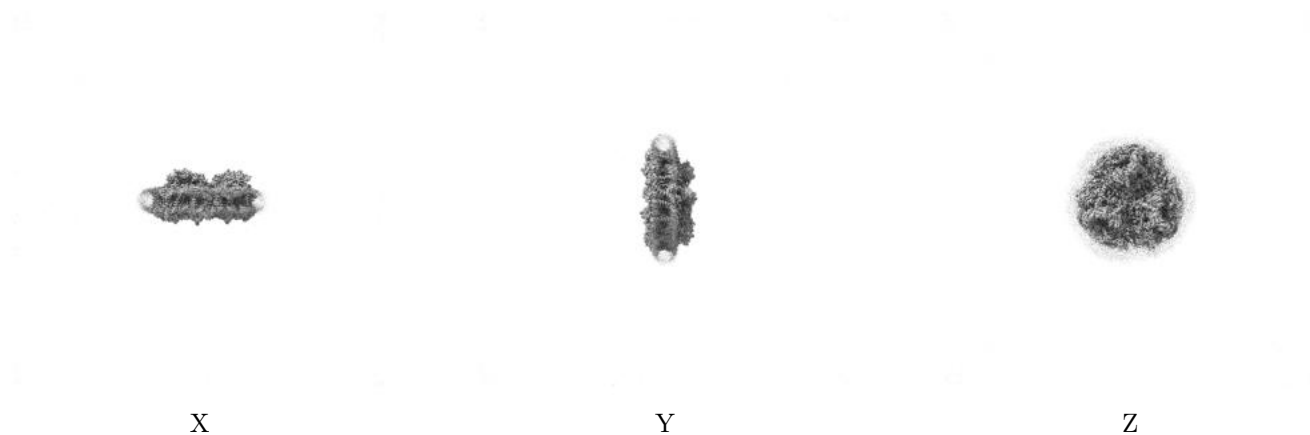
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.054. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

## 6.6 Mask visualisation [i](#)

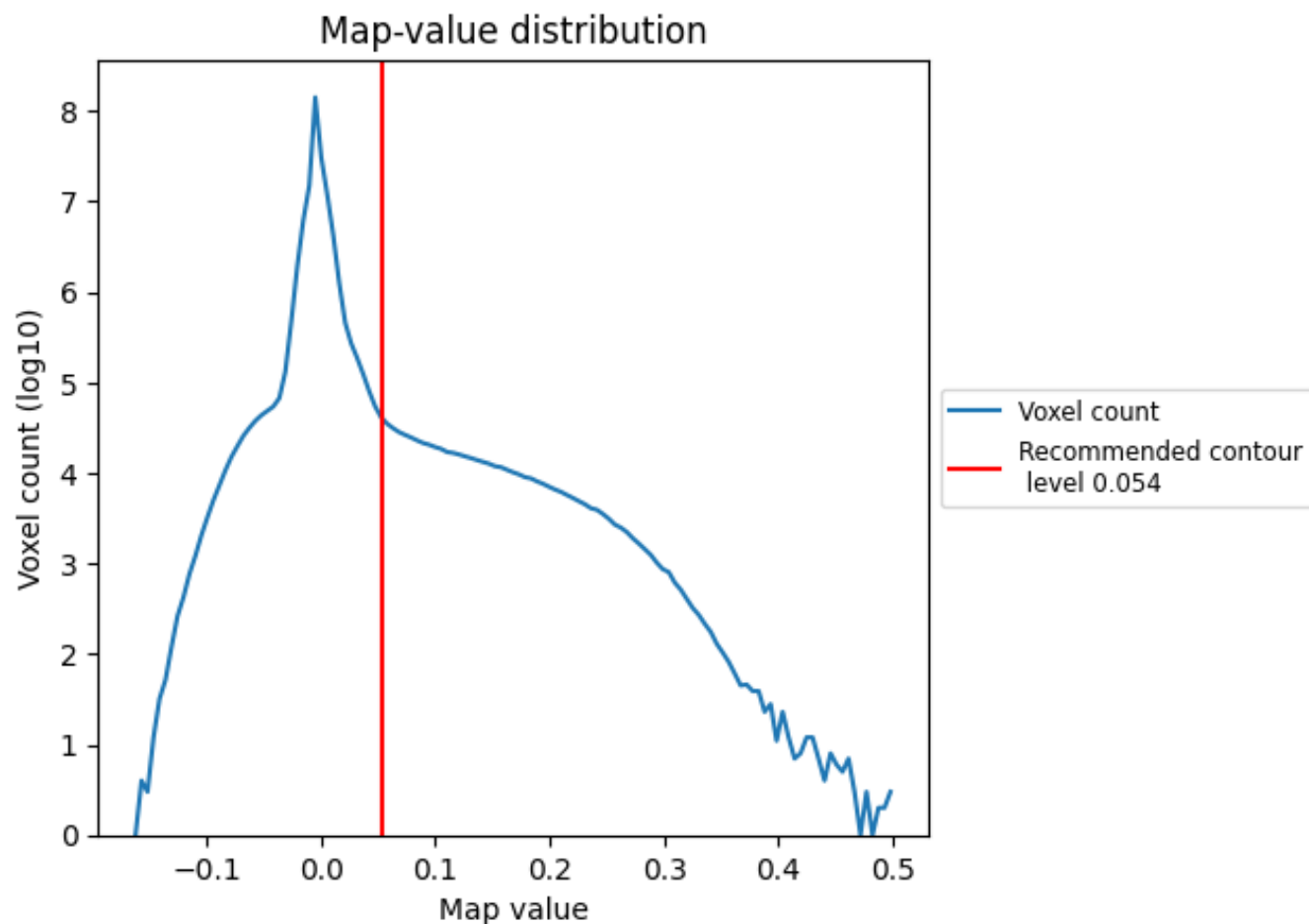
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

This section contains the results of statistical analysis of the map.

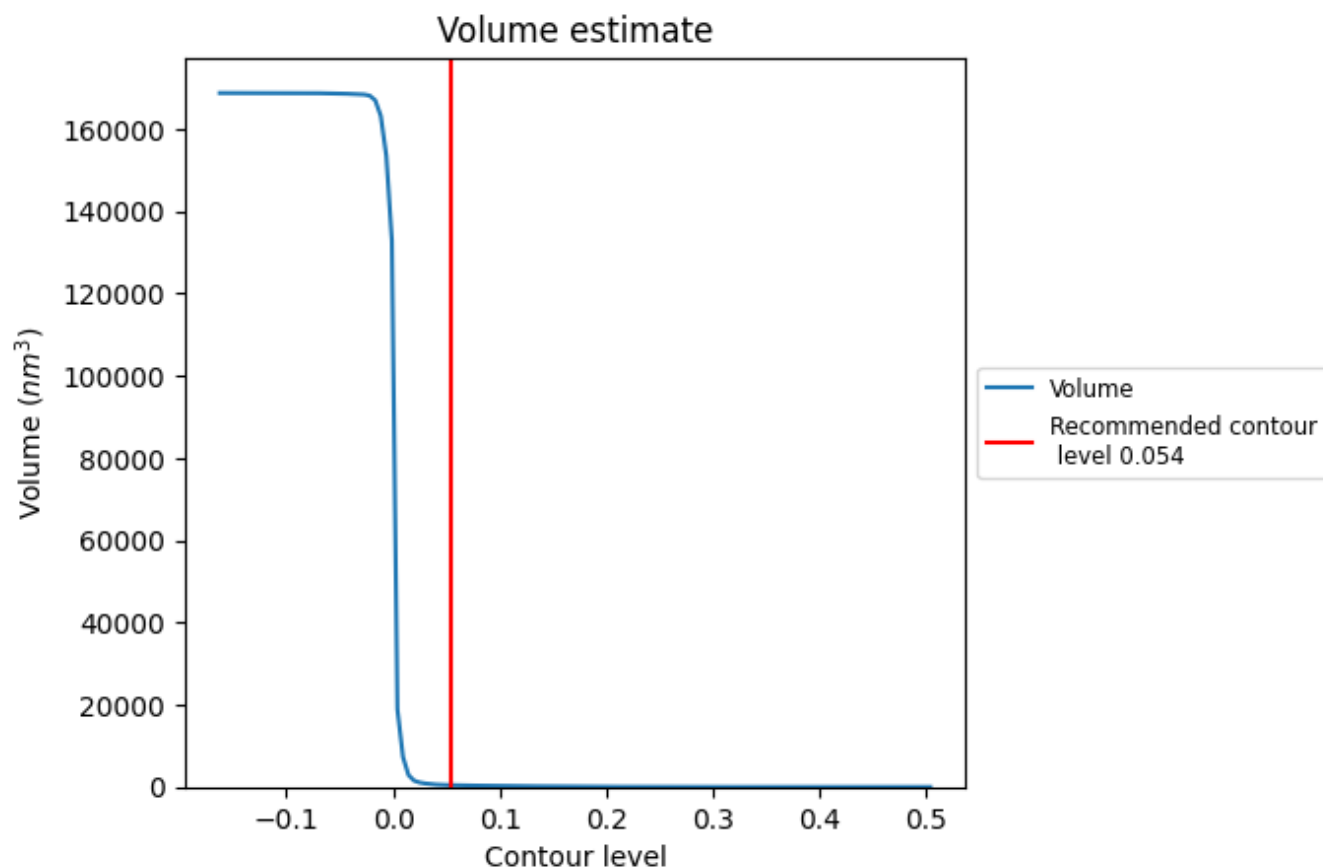
### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.



## 7.2 Volume estimate [i](#)

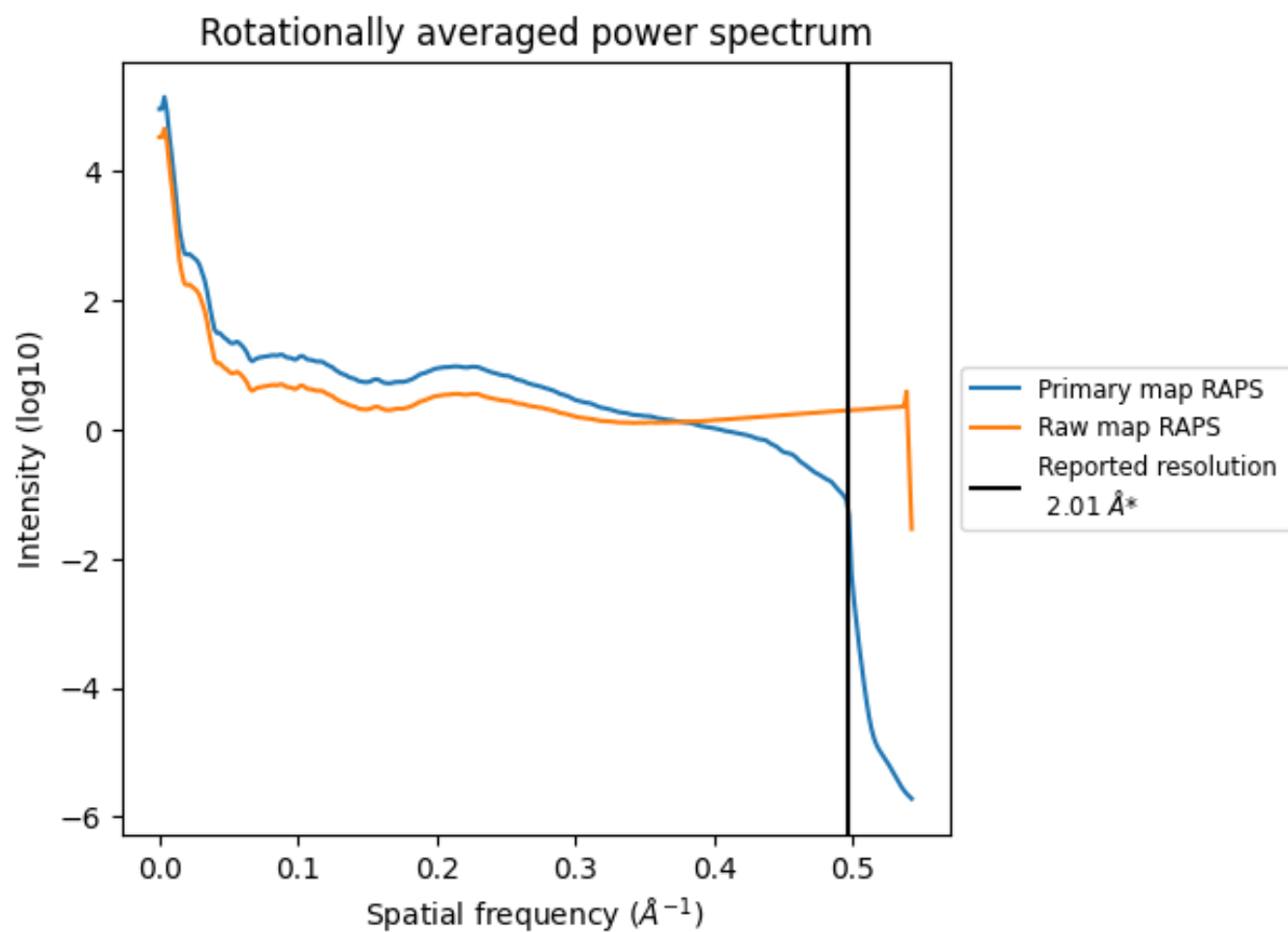


The volume at the recommended contour level is 439 nm<sup>3</sup>; this corresponds to an approximate mass of 396 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.



### 7.3 Rotationally averaged power spectrum ⓘ



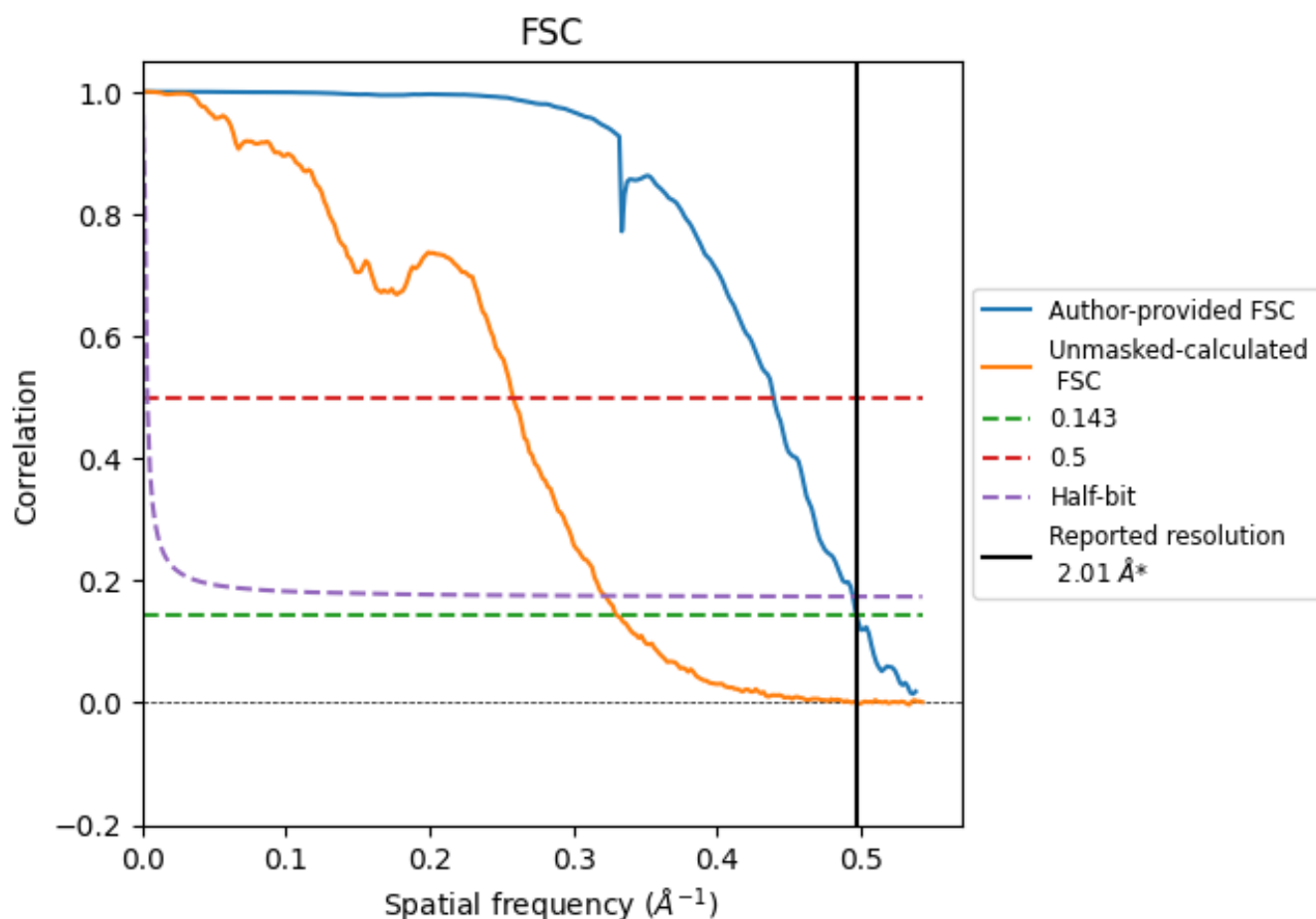
\*Reported resolution corresponds to spatial frequency of  $0.498 \text{ \AA}^{-1}$



## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.498 \text{ \AA}^{-1}$



## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.01	-	-
Author-provided FSC curve	2.01	2.27	2.02
Unmasked-calculated*	3.03	3.87	3.10

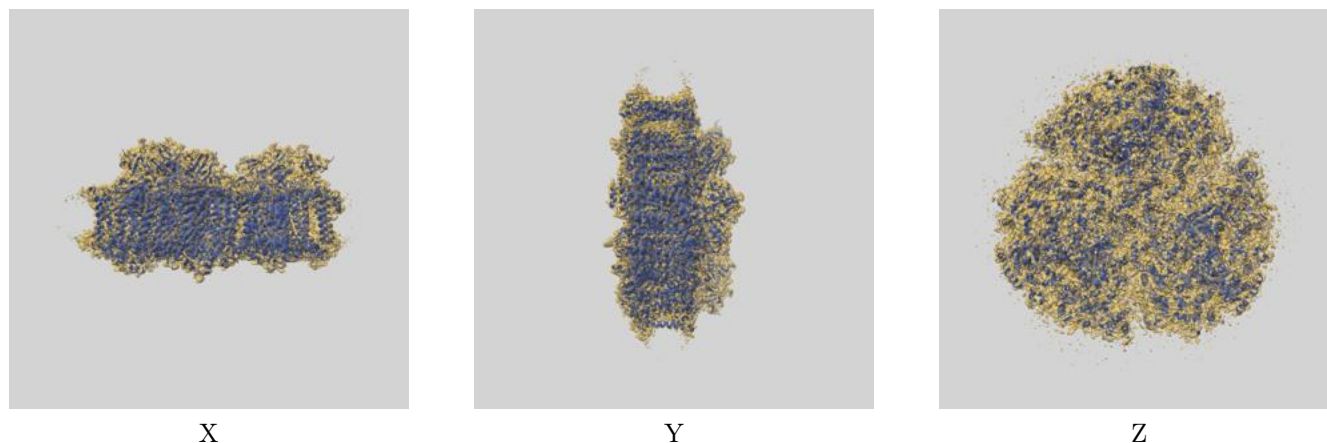
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.03 differs from the reported value 2.01 by more than 10 %



## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-50063 and PDB model 9EYS. Per-residue inclusion information can be found in section [3](#) on page [41](#).

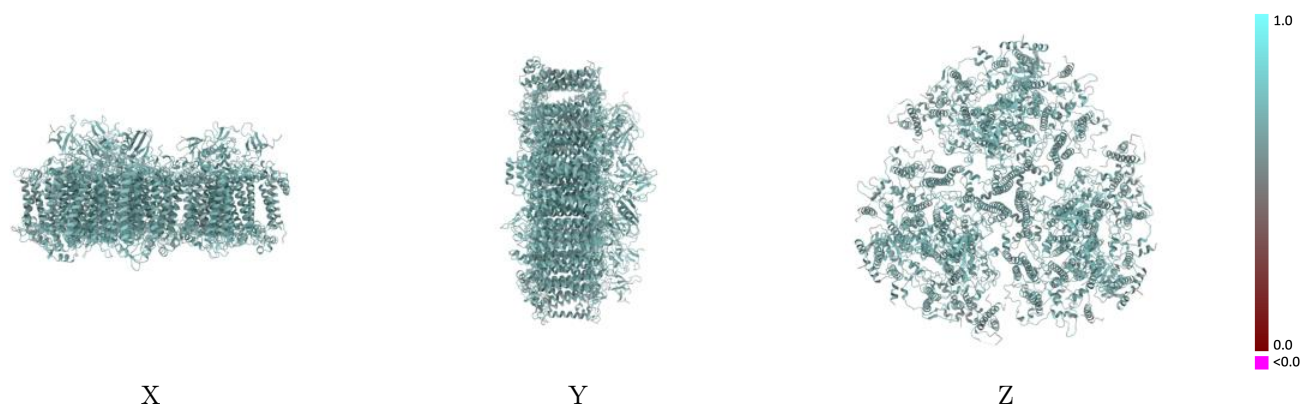
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.054 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

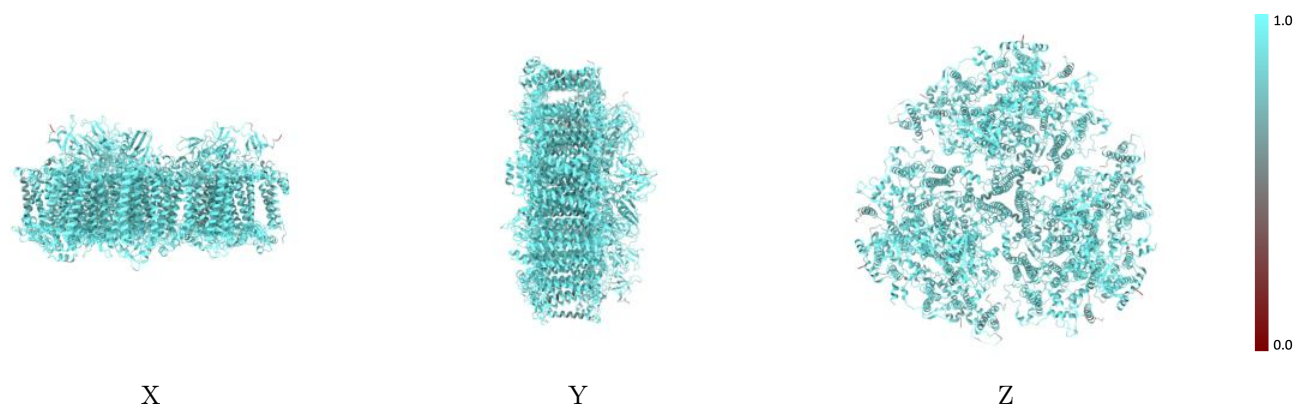


## 9.2 Q-score mapped to coordinate model [i](#)



The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

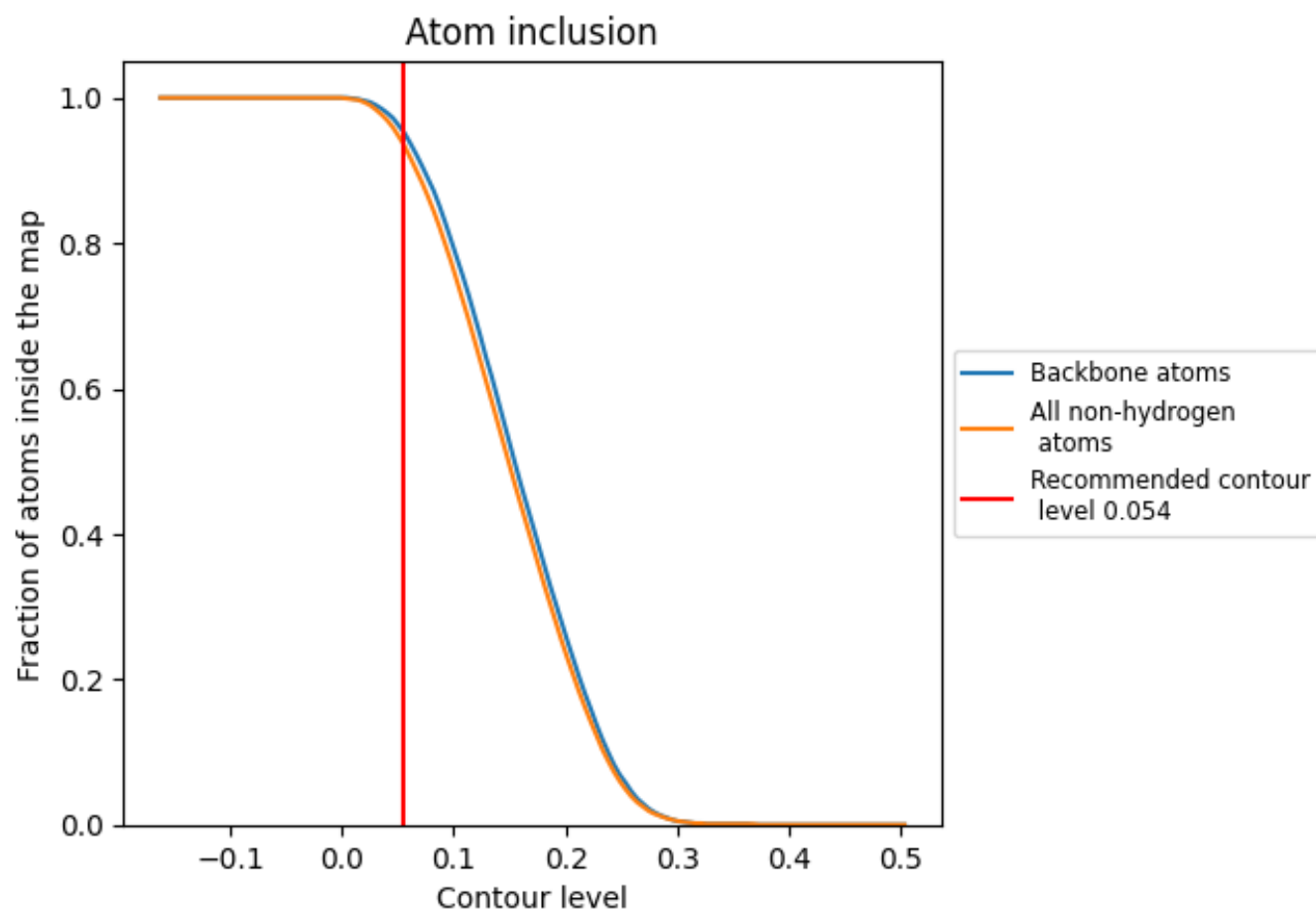
## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.054).



## 9.4 Atom inclusion [i](#)









































































At the recommended contour level, 96% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.



## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.054) and Q-score for the entire model and for each chain.




Chain	Atom inclusion	Q-score
All	 0.9390	 0.6720
A	 0.9470	 0.6750
B	 0.9540	 0.6780
C	 0.9900	 0.7050
D	 0.9570	 0.6740
E	 0.8950	 0.6460
F	 0.8920	 0.6430
I	 0.9590	 0.6890
J	 0.8860	 0.6330
K	 0.7630	 0.5740
L	 0.9590	 0.6910
M	 0.9230	 0.6640
N	 0.9460	 0.6760
O	 0.9530	 0.6790
P	 0.9920	 0.7070
Q	 0.9560	 0.6760
R	 0.8950	 0.6430
S	 0.8930	 0.6440
T	 0.9630	 0.6930
U	 0.8900	 0.6370
V	 0.7750	 0.5800
W	 0.9610	 0.6960
X	 0.7170	 0.5900
Y	 0.9230	 0.6650
Z	 0.7280	 0.5910
a	 0.9470	 0.6750
b	 0.9530	 0.6790
c	 0.9930	 0.7030
d	 0.9580	 0.6760
e	 0.8930	 0.6450
f	 0.9010	 0.6470
g	 0.9570	 0.6900
h	 0.8840	 0.6370
i	 0.7740	 0.5870
j	 0.9600	 0.6950



*Continued on next page...*



*Continued from previous page...*

Chain	Atom inclusion	Q-score
k	 0.9260	 0.6650
l	 0.7090	 0.5940